

# Computational analysis of N-methyltransferase enzymes from *T. elegans* and *Catharanthus roseus*

Matthew Richardson<sup>1</sup>

<sup>1</sup>University of New Brunswick

Vinblastine the anti-cancer drug comprised of a monoterpenoid indole alkaloid (MIA), is found, and collected primarily in the Madagascar periwinkle, *Catharanthus roseus*. With the large demand for effective cancer treatments, finding alternative plants that produce precursors of vinblastine has led to the investigation of *Tabernaemontana elegans*. Enzyme assays previously conducted revealed a more efficient production of vobasine when compared to *C. roseus*. However, due to the limitations of X-ray crystallography, the reasons for this discrepancy have remained largely unknown. To address this issue and better understand the enzymatic mechanisms that have led to this discrepancy between both N-methyl transferases, we made use of the Molecular Operating Environment (MOE) to generate homology models of each plant's enzymes using their amino acid sequences. Docking simulations were then performed on said models, placing their co-enzyme (S-adenosyl methionine) and ligand (perivine) into their active sites shedding light on the differences between both enzymes. Our computational analysis revealed a superior binding angle between the secondary amine of perivine and the methyl group attached to the sulfonium ion of SAM in the *T. elegans* model, caused by various side chains within its active site. This improved angle in theory allows for better methylation of perivine via an SN2 reaction, transforming the molecule into Vobasine. The findings from this research suggest a possible explanation for the enhanced production of vobasine observed in *T. elegans* compared to *C. roseus*. The study illuminates the potential of computational modeling when it comes to understanding enzymatic mechanisms and without a doubt will inform subsequent research concerning the optimization of vinblastine production.

## Affiliation

University of New Brunswick

# ADVANCED FORMULATION OF NANOGEL FOR CRYOPRESERVATION

Zeyaealdin Zarei<sup>1</sup>, Marya Ahmed<sup>1</sup>

<sup>1</sup>University of Prince Edward Island

*Cryopreservation* is a technique used to store cells and tissues at low temperatures to maintain their structure and functional integrity. This procedure usually incorporates cryoprotectants (CPAs), which prevent ice crystal formation and minimize cellular damage during freezing and thawing processes. CPAs achieve this by lowering the freezing point and reducing the effects of dehydration, facilitating successful cell revival after cryopreservation. However, common cryoprotectants, such as dimethyl sulfoxide (DMSO), are toxic when used at high concentrations and can have adverse effects. Therefore, serums such as fetal bovine serum (FBS) are needed to reduce toxicity, although increasing the risk of contamination and immunogenic responses to the cryopreserved samples. Hence, there is a need to explore non-toxic alternative materials to enhance the preservation of diverse biological materials, prompting this study's focus on nanogels. This study has focused on nanogels synthesized from vitamin B5 analogous methacrylamide (B5AMA) crosslinked with 3,9-Divinyl-2,4,8,10-tetraoxaspiro [5.5] undecane (OXAS) and divinyl sulfone (DVS) and characterized using dynamic light scattering (DLS) and nuclear magnetic resonance spectroscopy (NMR). These nanogels were then employed as CPAs to compare their efficiency in the cryopreservation of mammalian cells.

## **Affiliation**

University of Prince Edward Island

# Biochar and pyrolysis: A closer look at the Chartl

Crewe Macdonald<sup>1</sup>

<sup>1</sup>cape breton university

The transition away from the use of fossil fuels and environmentally unfriendly energy sources into cleaner, more sustainable energy sources are necessary for a brighter and healthier future for our planet. The development of renewable waste management techniques is important to accomplish this. Among these techniques is pyrolysis, which can be used to convert biomass waste into more useful materials like biochar. The MacQuarrie Group (or The CHArTI) focuses on organic materials research and performs pyrolysis on several forms of biomass waste such as woody, citrus, crab, seaweed, and pharmaceutical waste. The process of pyrolysis is the burning of biomass material in the absence of oxygen under nitrogen, and produces solid biochar, oils and gas. All these products are collected, characterized, and used for several applications such as waste management, agriculture, textiles, water remediation, catalysis, and metal recovery. This talk will serve as an overview of pyrolysis and the research conducted by The MacQuarrie Group at Cape Breton University (CBU).

## **Affiliation**

Cape Breton University

# Fish Oil as Fuel?

Angela Amati<sup>1</sup>

<sup>1</sup>Cape Breton University

The triglycerides found in biomass sources such as fish oils can be converted into a mixture of fatty acid methyl esters (FAMES), also termed “biodiesel” because of its physical similarities to petroleum diesel. This process is referred to as transesterification (TRE), which in the presence of a short-chain alcohol and a catalyst, the triglycerides present in any organic oil are converted into a mixture of FAMES. The use of a catalyst in this process aids in the speed of the reaction, and the use of calcium oxide (CaO) is preferred due to its catalytic, financial, and safety advantages. CaO can be obtained from crab waste, which is composed mostly of water, chitin, and calcium carbonate (CaCO<sub>3</sub>). By removing any hydration from the crab material and then calcinating the material, CaCO<sub>3</sub> can be converted into CaO. Fourier Transform Infrared (FT-IR) spectroscopy, X-ray Diffraction (XRD) spectroscopy, BET analysis, and elemental analysis was used to characterize the catalyst to ensure it was properly calcinated. Conditions for the TRE reaction include: 5.0 g fish oil, 30-40 mL methanol, 0.5-2.0 g catalyst-loading, 80 °C reflux temperature, and 2-4 hours reflux time. Nuclear Magnetic Resonance (NMR) spectroscopy was used to determine the %conversion from reactant to product using the integration of the methoxy group from the FAME at about 3.7 ppm and the  $\alpha$ -CH<sub>2</sub> group that is present in both the reactant and product at about 2.3 ppm. After the use of commercial CaO as a catalyst and a catalyst-loading of 0.5 g and a reflux time of 2 hours, a %conversion of 88%  $\pm$  7% was observed. Then with the use of the prepared crab material catalyst and a catalyst-loading of 2.0 g and a reflux time of 4 hours, a %conversion of 87%  $\pm$  2% was observed. The optimization of this process is important for the application of biodiesel in replacement of petroleum diesel since the international standard for biodiesel requires an above 96.5% FAME content.

## **Affiliation**

Cape Breton University

# Role of Peptide Architecture and Composition in Folic Acid Delivery

Vineet Kumar Mishra<sup>1</sup>, Marya Ahmed<sup>1</sup>

<sup>1</sup>University of prince edward isalnd

**CHEMCON 2024**

## Abstract

### Role of Peptide Architecture and Composition in Folic Acid Delivery

*Vineet Kumar Mishra & Marya Ahmed*

Cell-penetrating peptides (CPPs) are broadly recognized as efficient non-viral vectors for the internalization of essential macro and micronutrients, therapeutic oligonucleotides, and drugs in the living cells. These peptides can be cationic, amphipathic, or hydrophobic in nature. Advantages of peptide-based carriers over other delivery systems are their non-immunogenic and non-cytotoxic nature, stability under physiological conditions and rapid delivery of cargo into prokaryotic and eukaryotic cells. This study aims to investigate the role of peptide composition and architecture on folic acid delivery efficacies and their immunomodulatory outcomes in the presence of bacteria and virus challenge *in vitro*. For this purpose, a library of linear and cyclic peptides with cationic (TAT), amphipathic (KALA) and hydrophobic (C105Y) nature was synthesized and conjugated with folic acid. The successful synthesis of linear and cyclic peptides and corresponding conjugates was confirmed by mass spectrometry. CPPs were tested for their cellular uptake, enzymatic stability and bioavailability of folic acid in intestinal cells and macrophages. Our results indicate that compared to linear CPPs, cyclic CPPs are better internalized in cells and showed higher bioavailability as was demonstrated by the downregulation of folate receptors and by the evaluation of immunomodulatory activities of the conjugates.

## Affiliation

University of Prince Edward Island

# **Antibacterial Filters for Water Purification Developed from Plant Biomass Waste Stream**

Kevin Scotland<sup>1</sup>

<sup>1</sup>Cape Breton University

## **Antibacterial Filters for Water Purification Developed from Plant Biomass Waste Stream**

**Kevin Scotland**

There is a historic issue of boiled water advisories in Canada's northern Indigenous communities and burgeoning issue of the proliferation multi-drug resistance bacterial in water sources in Canada (for example Potlotek). A novel multistep synthetic approach is proposed for the development of quaternary amine polymer for the contact killing of bacteria in water sources, without the use of electricity. Our research program will develop a novel route to ethylenimines, which will be used to produce new secondary amines. These secondary amines will be cyclized to novel tetrahydroisoquinolines which will be quaternized and polymerized by Reversible Addition Fragmentation Chain Transfer (RAFT) reaction, on to the surface of a carbon source (for example Biochar). It has been demonstrated that this quaternary amine material is an aggressive antibacterial agent that does allow the bacterial present in the water source to acquire multi-drug resistance.

### **Affiliation**

Cape Breton University

# Phthalates in Focus: Roles, Risks, and Analysis

Jamey Toney-Gagne<sup>1</sup>, Madison Power<sup>1</sup>

<sup>1</sup>Cape Breton University

Phthalates are a group of synthetic phthalic acid esters (PAEs) used as plasticizers to make plastics more durable, help to dissolve other materials, hold fragrances, and facilitate uniformity of coatings. PAEs added to polymeric material to enhance properties are not chemically bound and readily leach into the environment. Despite PAEs being pervasive in the environment, the full extent of leaching into different matrices is not known as comprehensive extraction and sensitive detections methods require further optimization at relevant PAE concentrations. It is important for PAEs to be monitored as some have been classified as endocrine disrupting chemicals (EDCs), suspected carcinogens, and acutely toxic to aquatic organisms. The length of the carbon side chain on PAEs determines whether they are categorized as low molecular weight (LMW) PAEs, transitional PAEs, or high molecular weight PAEs. The category of PAE and route of entry determine the possible adverse effects on humans and the environment. Current environmental monitoring of PAEs in Canada focuses on one PAE, Diethylhexyl phthalate (DEHP), that can exist in harmful concentrations in the environment due to its widespread applications. Alternatives to PAEs exist but are presented with different challenges that lead to PAEs continuously being used. Small concentrations of phthalates, micrograms per litre or parts per billion (ppb w/v), can be detrimental to both humans and the environment. A comprehensive extraction method that is easy, efficient, and cost-effective is needed to make environmental monitoring of PAEs more accessible. Magnetic dispersive solid-phase extraction (MDPSE) will be explored as a method of PAE extraction from water samples. Gas chromatography tandem mass spectrometry (GC-MS/MS) as the method of detection of PAEs has been under optimization for analysis of select PAEs at the ppb level due to its sensitivity, high selectivity, and high resolution. Thus, this presentation provides a comprehensive overview of PAEs, their effects on humans and environment, their reasons for obscurity in environment, and advancements in standard analytical methods.

## **Affiliation**

Cape Breton University

# Functionalization of Biochar with Thiourea for Cadmium Adsorption

Ava Graham<sup>1</sup>, Stephanie MacQuarrie<sup>1</sup>

<sup>1</sup>Cape Breton University

Cadmium is a naturally occurring metal that is disturbed from the environment as a result of human activity, such as mining or smelting. This can result in the contamination of air, water, and eventually crops. Exposure to cadmium can lead to a series of adverse health effects, such as osteoporosis and cardiac failure. Therefore, it is essential to monitor cadmium levels, especially in high-risk areas, and limit exposure as much as possible. Biochar is a carbon-rich material which may be used as a method of limiting cadmium exposure. Although it has adsorptive properties on its own, it can be chemically functionalized to bind to cadmium, thus giving it the potential to remove this heavy metal from the environment. Biochar was created through the pyrolysis of woody biomass and oxidized using the Modified Hummers Method. Silyl thiourea was then synthesized using (3-Aminopropyl)triethoxysilane (APTES) and phenyl isothiocyanate, and characterized using both proton-NMR and C-NMR. Thiourea has a high affinity for cadmium binding as a result of its two nitrogen atoms and its sulfur atom. Therefore, functionalizing oxidized biochar with silyl thiourea may be able to remove cadmium from the environment, in an effort to remediate cadmium contaminated areas.

## Affiliation

Cape Breton University



# **A Song of Fruit and Fire**

Madeline Marinelli<sup>1,2</sup>, Stephanie MacQuarrie<sup>1</sup>, Michael Katz<sup>2</sup>

<sup>1</sup>Cape Breton University, <sup>2</sup>Memorial University

The primary focus for this project is on repurposing fruit waste, specifically banana peel, orange peel, and pineapple leaf, through its conversion into biochar, a carbon-rich material produced via biomass thermochemical conversion. The goal is to address the environmental challenge posed by significant annual accumulation of fruit waste from processing industries.

This study contributes to advancing sustainable waste management practices by leveraging the value of fruit waste in biochar production.

While past studies have successfully produced biochar from fruit waste, this research emphasizes the influence of pyrolysis conditions and biomass composition on the variability of biochar properties.

Through analytical techniques, the aim is to comprehensively study the organic and inorganic properties, surface area, and micropore volume produced within the biochar under varying pyrolysis conditions, and to highlight the unique properties of biochar and its potential applications beyond agriculture, particularly in mitigating odor emissions.

## **Affiliation**

Cape Breton University and Memorial University

# Tailored Magnetic Nanocomposites for Co-Recovery of Metals from Wastewater

Marzieh Baneshi<sup>1</sup>

<sup>1</sup>Cape Breton University

Human activities generate significant quantities of wastewater containing considerable amounts of metals, presenting both environmental challenges and economic opportunities. Conventional methods for metal recovery often face limitations in efficiently extracting multiple metals simultaneously. In response, this research program focuses on the development of custom-tailored magnetic nanocomposites (MNCs) designed to selectively capture and separate target metals from complex aqueous matrices. Leveraging the Differential Magnetic Catch and Release (DMCR) effect, wherein MNCs exhibit varying responses to external magnetic fields, this research aims to achieve unprecedented levels of selectivity and efficiency in co-recovering various metals.

The tunability of MNCs enables precise control over their saturation magnetization, while strategic engineering and functionalization enhance their ability to target specific metals for extraction. By harnessing these capabilities, the research aims to enable the concurrent removal and recycling of diverse metals from industrial wastewater streams. This approach not only addresses challenges associated with metal co-extraction but also offers a sustainable and cost-effective solution for valorizing wastewater and reclaiming valuable resources.

## **Affiliation**

Cape Breton University

# Terpyridine Supported Phosphorus (III) Dication Transfers and the Related Homologous Series

William P. Howlett<sup>1</sup>

<sup>1</sup>Dalhousie University

Recently, the transfer of  $XP^{2+}$  ( $X = Cl, Ph$ ) fragments to other ligands has been effected by our group using the all L-type NNN ligand system BZIMPY. Commercially available ligands terpyridine (terpy) and bipyridine (bipy) possess a similar all L-type motif to BZIMPY that may enable a similar ability to transfer the  $XP^{2+}$  group to other ligands or access otherwise difficult chemistry without requiring an exotic ligand. Phenyl phosphorus (III) dications using these ligands have additionally already been shown by the Stephan group to engage in Lewis acid catalysis such as in hydrodefluorination of C-F bonds<sup>1</sup> and hydrosilylation of olefins and carbonyls.<sup>2</sup> Transfer of the  $PhP^{2+}$  moiety from  $[PhP(terpy)][OTf]_2$  has been successfully performed for some L-type donor ligands. The heavier element analogues in the homologous series of  $[PhPn(terpy)][OTf]_2$  ( $Pn = As, Sb, Bi$ ) have been synthesized and characterized, and reactivity studies are to be performed. A modified variant of terpy was also used in synthesizing the phosphorus dication,  $[PhP((p\text{-tolyl})terpy)][OTf]_2$ , in which the *para*-position in the central pyridine ring is substituted with a *p*-tolyl group, blocking Lewis acidity known to occur at this site in the unsubstituted complex.

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## Affiliation

Dalhousie University

# A New Route to Functionalize Biochar

Alyssa Burke<sup>1</sup>, Dr. Stephanie MacQuarrie<sup>1</sup>

<sup>1</sup>Cape Breton University

Biochar is a carbon-rich porous material that has applications in waste management, materials such as insulation and catalysts, and agriculture. This material is formed via pyrolysis. Pyrolysis is a method of heating biomass under inert conditions, resulting in the generation of biochar, oil, and gas. This biochar can be functionalized, which is an important topic in current literature. This involves adding new functional groups to the surface of biochar; which can help enhance the adsorption for specific molecules. The addition of surface functionality onto the biochar that can undergo cross coupling reactions, advances the scope of surface functionalization of biochar by allowing us to attach a multitude of functional groups on biochar. This study will focus on the cross-coupling reactions of brominated biochar with pinacolborane. To achieve this, biochar would first have to be brominated. A bromination procedure with bromine and dichloromethane was performed resulting in a 95% recovered yield of the woody biochar. Fourier-Transform Infrared Spectroscopy showed the presence of a peak at  $701.88\text{ cm}^{-1}$  in the IR spectrum, suggesting that the material was brominated. The BET surface area showed an increase of  $18.7\text{ m}^2/\text{g}$ , demonstrating that bromination took place and did not severely affect the surface area of the material.

## Affiliation

Cape Breton University

# Maskwio'mi - a Traditional Mi'kmaw Skin Medicine: Study of the Sources of the Pharmacologically Active Compounds

Alexa Stermann<sup>1</sup>

<sup>1</sup>Cape Breton University

Worldwide, over 2 billion people suffer from chronic skin conditions such as eczema and psoriasis. Birch products have been used by cultures around the globe for many medicinal purposes. The Mi'kmaq people of Atlantic Canada have the natural skin remedy of maskwio'mi (maskwi = birch bark; o'mi = gathering/oil) which is a viscous extract of the paper birch (*Betula papyrifera*) obtained in a thermolytic pyrolysis process and formulated into creams.

Preliminary chemical analyses using GC-MS and UPLC-MS show that maskwio'mi is a highly complex organic matrix with over 100 compounds. Antibacterial studies reported that the extract is effective against Gram-positive and Gram-negative bacteria. The current hypothesis is that maskwio'mi contains a wide range of pharmaceutically active compounds which originated in the bark a priori or were formed during pyrolysis, or a combination of both pathways.

The majority of biomass in birch bark is made up with cellulose, hemicellulose and lignin with additional secondary metabolites. This study is comparing the pyrolytic extracts of the whole bark with that of cellulose, hemicellulose, and lignin. The obtained extracts are analyzed using GC-MS. Antimicrobial activity of extracts of each biomass component is evaluated against selected pathogens, including *Escherichia coli* and *Staphylococcus aureus*.

## **Affiliation**

Cape Breton University

# Synthesis, Reactivity, and Electrochemical Studies of Bis(2-(dimethylaminomethyl)ferrocenyl)bismuth Chloride

Emily England<sup>1</sup>, Glen Briand<sup>1</sup>, Suhjung Chun<sup>1</sup>, Gregory Sandala<sup>1</sup>, Tanner George<sup>2</sup>, Jason Masuda<sup>2</sup>

<sup>1</sup>Mount Allison University, <sup>2</sup>Saint Mary's University

Expensive and toxic precious metal-based organometallic compounds are widely used as redox catalysts for chemical transformations important to the pharmaceutical and fine chemical industries. The current emphasis on “Green Chemistry” has created a demand for alternative chemical compounds that mitigate the high cost and harmful environmental effects of current approaches. Organometallic compounds of base main group metals, such as bismuth, offer an affordable and environmentally benign solution to this problem. Bismuth is most stable in the +3-oxidation state, although its other oxidation states can be accessed under highly specific conditions. Consequently, redox activity is not typically inherent to bismuth compounds, though it can be facilitated through use of redox-active ligands such as ferrocene; previous studies have shown ferrocenyl bismuth compounds exhibit well-defined, reversible redox processes. The current study aims to synthesize and characterize bis(2-(dimethylaminomethyl)ferrocenyl)bismuth chloride, a novel compound that is a potential green alternative to transition metal catalysts. To understand the scope of its efficacy to catalyze industrially relevant chemical transformations, the chemical reactivity and electrochemical properties of the compound will be studied.

## Affiliation

Mount Allison University

# Enhanced Copper Durability with N-Heterocyclic Carbene Monolayers

Mary Stackaruk<sup>1, 2, 3, 4, 5, 6</sup>

<sup>1</sup>Surface Science, <sup>2</sup>Spectroelectrochemistry, <sup>3</sup>Surface-enhanced Raman Spectroscopy, <sup>4</sup>N-Heterocyclic carbene, <sup>5</sup>Organic Synthesis, <sup>6</sup>Aqueous electrochemistry

Copper is an abundant and low-cost metal that is widely used in the electronic industry and exhibits one of the highest conductivities. In addition to copper use in the electronic industry, copper can be used for diagnostic sensing in spectroelectrochemistry and in synthetic catalysis. Unfortunately, copper readily oxidizes in acidic, high thermal, and even in ambient conditions. N-heterocyclic carbene (NHC) self-assembled monolayers are known as a highly stable cyclic organic compounds that are resistant to the same conditions that make copper corrode. NHC SAMs have been formed on copper-coated screen-printed electrodes (CuSPEs) through aqueous electrochemistry and the formation of the monolayer has been monitored using electrochemical surface-enhanced Raman spectroscopy. NHC-coated CuSPE were immersed in 0.1 M NaOH to fast-track the oxidation of the copper surface. Results showed that after 14.5 hours in oxidizing conditions, the NHC-coated CuSPE had only 3.02% total oxides vs. an unprotected CuSPE with 25.94% oxides.

## Affiliation

Saint Marys University

# Production of reactive oxygen species by e-cigarette smoke in surrogate lung fluid

Moriah Hennessey<sup>1</sup>, Jenny Wong<sup>1</sup>

<sup>1</sup>Mount Allison University

E-cigarettes, also known as vapes, are electronic nicotine delivery devices marketed as a healthy alternative to traditional cigarettes. Recently, the use of e-cigarettes among Canadian youth has recently surpassed that of traditional cigarettes. Previous studies have shown that e-cigarette smoke contains many of the harmful substances present in traditional cigarettes. In addition, e-cigarette smoke has been shown to increase the presence of reactive oxygen species (ROS) in lung cells, causing oxidative stress that can lead to various pulmonary and cardiovascular diseases. The current study examines how filament resistance and power settings, both user-defined parameters, affect ROS concentrations produced when e-cigarette smoke interacts with a surrogate lung fluid (SLF) containing antioxidants found in human lungs. E-cigarette smoke was generated using settings at both recommended by the user-manual and those that exceed recommendations. Following collection, the e-cigarette smoke was introduced to SLF, and hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) production was quantified using an acellular 2,7-dichlorofluorescein-horseradish peroxidase (DCFH-HRP) assay. Results indicate that as the filament wattage increased, the H<sub>2</sub>O<sub>2</sub> concentration increased. Notably, H<sub>2</sub>O<sub>2</sub> was still produced at the recommended settings. It was also found that ROS were not present in the smoke alone but instead, are produced through reactions of smoke components with SLF antioxidants. This study provides insight into how the user behaviour can influence of an e-cigarette toxicity and highlights potential areas for modifications in e-cigarettes design and use to reduce health risks.

## **Affiliation**

Mount Allison University



# Acute Toxicity of Brake Pad Wear on Brook Char Gills (*Salvelinus fontinalis*)

Zoë LindenSmith<sup>1</sup>, Jenny Wong<sup>1</sup>, Tyson MacCormack<sup>1</sup>

<sup>1</sup>Mount Allison University

Non-exhaust emissions account for half of traffic-derived particulate matter (PM) emissions, with 55% by mass of this non-exhaust emission originating from brake pad wear (BPW). Various formulations of brake pads, which are aerosolized to form atmospheric PM during the braking process, differ in chemical composition and efficacy. BPW PM contains metal species such as iron and copper that are known to induce toxicity through reactive oxygen species (ROS) production, and can disperse via the atmosphere, eventually depositing in aquatic ecosystems. This study directly compares the toxicity of two formulations of BPW—ceramic and semi-metallic—in aquatic ecosystems. Exposures were conducted using isolated perfused gills, from brook char (*Salvelinus fontinalis*), a primary site of aquatic exposure, with both physical and chemical endpoints measured to ascertain potential mechanisms of BPW toxicity. Ceramic samples contained 22 ppb of copper and induced oxidative membrane damage with 1.5 times more lipid peroxidation than their respective control. Surprisingly, iron and copper were undetectable in semi-metallic BPW samples, and did not induce significant oxidative damage compared to their respective control. Both ceramic and semi-metallic samples induced physical damage to the gill epithelium, triggering an inflammatory immune response, as qualitatively assessed by SEM imaging. These results provide evidence of physical and chemical BPW-induced damage to gill tissue under environmental conditions, which has important implications for aquatic ecosystems as this damage has unknown long-term effects on organisms.

## Affiliation

Mount Allison University

# A Cyclophane Approach to the Synthesis of Open Geodesic Polyarenes Exhibiting Fullerene-type Chemistry

Samuel Chaulk<sup>1</sup>

<sup>1</sup>Memorial University of Newfoundland

A Cyclophane Approach to the Synthesis of Open Geodesic Polyarenes Exhibiting Fullerene-type Chemistry

Samuel R. Chaulk, Graham J. Bodwell

*Chemistry Department, Memorial University of Newfoundland,*

*45 Arctic Avenue, St. John's, NL, Canada, A1C 5S7*

E-mail: srchaulk@mun.ca

Geodesic polycyclic arenes (GPAs) are a class of polycyclic aromatic hydrocarbons (PAHs) that contain one or more five-membered (or smaller) rings resulting in non-planar equilibrium state [1]. The smallest GPA that exhibits fullerene-type chemistry is diindeno[1,2,3,4-*defg*;1',2',3',4'-*mno*p]chrysene (**1**), which undergoes addition reactions at the central carbon atoms to relieve pyramidalization strain as they transform from  $sp^2$  to  $sp^3$  hybridization [2]. The high strain energies of these nonplanar GPAs means that their synthesis is challenging. Consequently, previous syntheses of these GPAs frequently require the use of high energy methods such as flash vacuum pyrolysis (FVP) at temperatures exceeding 1000 °C [2,3]. The use of such conditions severely limits the presence of non-participating functional groups.

The goal of this work is to apply established synthetic methodology used in the synthesis of a wide range of small cyclophanes to the synthesis of difluoreno[2,1,9,8,7-*defg*;2',1',9',8',7'-*mno*pqr]naphthacene (**3**). The key feature of this approach is that incremental increases in strain energy will be introduced and the development of aromatic stabilization energy (ASE) will be used to offset developing strain in the later stages of the synthesis [4]. Initial work has been aimed at the synthesis of 2,2',7,7'-tetrakis(bromomethyl)-9,9'-bifluorene (**2**), with current work focused on the synthesis of

dispiro[2,2',7,7'-fluorenetetraaldehyde][1.3.2]dioxadimethylsilole (**3**).

Figure 1: Smallest GPA with fullerene character (**1**) and retrosynthetic analysis of GPA (**4**)

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## Affiliation

Memorial University of Newfoundland

# Functionalization of Biochar with MPTMS for Gold Adsorption

Brandon MacDonald<sup>1</sup>, Stephanie MacQuarrie<sup>1</sup>, Ali Shafiee<sup>2</sup>

<sup>1</sup>Cape Breton University, <sup>2</sup>Trent University

Gold is a precious metal used in a wide variety of applications including jewelry, electronics, medicine, and chemical systems. The recovery of gold is a complex, expensive, and waste generating process. One method chemically that is considerable for gold recovery is using a Sulfur containing reagent being impregnated onto a source such as activated carbon. Using a Sulfur containing group such as 1-methyl-5-mercapto-1,2,3,4-tetrazole [MMT], it was found to have high gold recovery with concentrations of gold ranging from 10 to 100 mg/L of 79.3% at high concentrations and 93.7% at lower concentrations<sup>1</sup>. Through the use of Biochar, a carbon-rich, porous material that is made through thermochemical conversion of waste materials such as crab, pharmaceuticals and woody biomass, a method for gold recovery could be developed in solution. With the use of a modified hummers method, it is possible to oxidize the biochar with groups such as epoxide, carbonyl, carboxyl, and hydroxyl. These functional groups allow for further functionalization using (3-Mercaptopropyl) trimethoxysilane [MPTMS] anchoring onto the surface of the Biochar. This provides an alternative method for gold adsorption due to the strong electron affinity between gold and Sulfur.

## Affiliation

Cape Breton University

# From Sea to "C"atayst: Calcium Carbonate-Rich Crab Shell Biochar

Judith MacInnis<sup>1,2</sup>, Christina Bottaro<sup>1</sup>, Stephanie MacQuarrie<sup>2</sup>

<sup>1</sup>Memorial Univeristy of Newfoundland, <sup>2</sup>Cape Breton Univeristy

Over 1.8 million tons of seafood waste is generated annually and disposed of in landfills and the ocean. An alternative to the disposal of fishery waste is needed to eliminate the issues that arise due to the disposal of these materials. Studies have been carried out to provide environmentally friendly and value-added applications for fishery waste, one specific area involves the conversion of this waste to biochar. Biochar has been widely used as a support for metals in heterogenous catalysis, due to its feedstock availability, larger surface area, low cost, and stability in both acid and base media.

Crab shell biochar is rich in calcium carbonate, however, very little is known about the carbon in this crab shell biochar. This study investigates the demineralization of crab shell biochar (CSB) with the organic acid, citric acid, to remove carbon dioxide, as well as the characterization of remaining the carbon/calcium-salt. This project also investigates the applications of calcium citrate-rich biochar (CSBCA) as a heterogeneous catalyst support for Ni/Cu hydrodeoxygenation of vanillin, which will be used as a model for improving biofuel. We will then show that this biochar could also be used as a support for the Ni reduction of Cr (VI) to Cr (III); as well as a reusable catalyst for the catalytic pyrolysis of woody and seaweed biomasses which will produce biochar with increased surface area and increased porosity.

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## Affiliation

Memorial University of Newfoundland

# Examining Gold-Nanocluster-Allergen Bioconjugates for Immunotherapy Treatment

Victor Martinez Macias<sup>1</sup>, Alexander Foo<sup>1</sup>, Geniece Hallett-Tapley<sup>1</sup>

<sup>1</sup>St. Francis Xavier University

Functionalized gold nanomaterials have garnered considerable attention in modern medicine, establishing use in biosensors, imaging, biolabeling, and cancer therapies to name a few. Among these various nanostructures, gold nanoclusters (AuNC) have shown promising biological properties and photochemical activity. The present work is focused on developing a novel immunotherapy treatment to alleviate food allergies through coupling allergenic proteins onto AuNC. Here, Hen Egg White Lysozyme (Lys), a major allergen from eggs, was coupled to AuNC. The formation of Lysozyme-nanocluster bioconjugates (Lys-AuNC) was confirmed using fluorescence emission spectra. Further spectroscopic studies, coupled with Dynamic Light Scattering (DLS) and circular dichroism (CD) demonstrate that Lysozyme undergoes a drastic structural change upon AuNC conjugation. Denaturing curves obtained using tryptophan fluorescence showed a decrease in thermal stability compared to the native protein. Together, these results position Lys-AuNC as a promising immunotherapeutic compound: the changes in Lysozyme structure observed upon nanocluster formation could inhibit recognition by the host's antibodies - reducing the possibility of anaphylaxis upon administration. The reduction in thermostability could further reduce the allergenicity of AuNC-conjugated Lysozyme, further enhancing its safety and efficacy as an immunotherapeutic. Finally, the AuNC-bioconjugate technique can be easily applied to other allergen systems, allowing for its application against a diverse array of food allergens.

## Affiliation

St. Francis Xavier University

# Bismuth and Germanium Metal Complexes and Cations Stabilized by Bulky Cyclopentadienyl Complexes

Deana Symes<sup>1</sup>, Thai Do<sup>1</sup>, Tanner George<sup>1</sup>, Jason Masuda<sup>1</sup>

<sup>1</sup>Saint Mary's University

A series of novel cyclopentadienyl (Cp) bismuth and germanium metal complexes were prepared by using the sterically bulky 2,6-bis(2,4,6-trimethylphenyl)phenylcyclopentadienyl (<sup>TerMes</sup>Cp) ligand. Due to the steric demands of the <sup>TerMes</sup>Cp ligand, Cp-Metal-Aryl interactions may be promoted, stabilizing potentially unique metallic environments that can be further investigated. Mono-, bis-, and tris-<sup>TerMes</sup>Cp metal complexes were prepared by reacting <sup>TerMes</sup>Cp-K with the metal halides: GeCl<sub>2</sub> and BiI<sub>3</sub>. In some cases, stabilizing aryl interactions with the mesityl ring of the <sup>TerMes</sup>Cp ligand are present. Upon further reactivity, cationic germanium species [<sup>TerMes</sup>CpGe][GaCl<sub>4</sub>] and [<sup>TerMes</sup>CpGe][B(3,5-CF<sub>3</sub>-C<sub>6</sub>H<sub>3</sub>)] were synthesized by chloride abstraction of the germanium chloride using GaCl<sub>3</sub>, or by metathesis with Na[B(3,5-CF<sub>3</sub>-C<sub>6</sub>H<sub>3</sub>)] respectively.

## Affiliation

Saint Mary's University

# Modulating chitin synthesis in marine algae with iminosugars obtained by SmI<sub>2</sub> and FeCl<sub>3</sub>-mediated diastereoselective carbonyl ene reaction

Andreas Greulich<sup>1</sup>

<sup>1</sup>University of Stuttgart

Polyhydroxylated piperidines, so called iminosugars, are of particular interest due to their structural similarity with monosaccharides. Many of them serve as glycomimetics and inhibit or manipulate enzymes of the carbohydrate metabolism. The biological impact of these enzymes, e.g. glycosyl hydrolases that are involved in quality control and secretion pathways, make them interesting targets for treatments of diseases and infections. But due to their stereochemical structure (several stereogenic centers, proximity of polar groups) the synthesis of iminosugars is rather challenging. We decided to use a reported (by us, extended by Snaith) Lewis acid-catalyzed carbonyl ene reaction on amino acid derived aldehydes to get access to different diastereomers. In addition to classic Lewis acids we utilized SmI<sub>2</sub> since no reports for its use in carbonyl ene cyclizations towards piperidines had been published. We were able to synthesize differently modified piperidines based on L- and D-amino acids with high diastereomeric ratios. SmI<sub>2</sub> showed superior reaction control over FeCl<sub>3</sub> and MeAlCl<sub>2</sub>. Additional modification of the gained piperidines to polyhydroxylated scaffolds with different stereochemistry is shown to work too.

Iminosugars have been reported to interfere with glycosyltransferases, e.g. chitin synthases, too. A variety of iminosugars has been investigated as chitin synthase inhibitors *in vitro*. However, quantitative *in vivo* studies have not been reported. We established a new biological test system based on the algae *Thalassiosira rotula*. A quantitative analysis of the chitin synthesis of the algae can be performed *in vivo* under the light microscope. Selected piperidines were deprotected, tested for cytotoxicity and afterwards used in studies with the algae. The samples showed no cytotoxicity. The chitin synthesis studies showed a significant increase of chitin length during tests with the L-isoleucin derivatives. The amino acid residue seems to be the directing structure, not the different functionalization patterns. In addition the tests showed, that iminosugars can not only inhibit the chitin synthase but also stimulate it.

## Affiliation

University of Stuttgart



# Photocatalytic Hydrogen Generation Using Heterogeneous Nanocomposites

Lauren Gatto<sup>1</sup>, Geniece Hallett-Tapley<sup>1</sup>

<sup>1</sup>StFX University

Green chemical pathways are highly desired in alternative fuel generation. Solar, wind and hydrogen (H<sub>2</sub>)-derived methods can exploit environmentally favourable resources that limit climate drawbacks during power-generation. Of these, H<sub>2(g)</sub> is an ideal energy source given its recognized large energy capacity and absence of green house gas emissions. However, extensive development of H<sub>2</sub> fuel cells has been constrained by the energy cost associated with traditional methods of formation (*i.e.*, water electrolysis), but its large energy costs contradict the clear environmental benefit of H<sub>2</sub> fuel design.<sup>1</sup>

Photocatalysis has garnered considerable attention as an alternative means of H<sub>2</sub> generation. Moreover, the design of heterogenous catalysts introduces recoverable and reusable materials and limits additional environmental and chemical waste. Metal organic frameworks (MOF), specifically those comprised of zirconium metal centers, and metal oxide semiconductors (MO) both possess characteristics valuable for photocatalytic H<sub>2</sub> fuel design. In particular, MOF/MO hybrids have shown promise in hydrogen evolution reactions (HER),<sup>2, 3</sup> Decoration of MOF/MO using gold, copper, platinum, or nickel nanospecies (NS) may extend the light activated state, further improving photocatalytic activity.

The current contribution will present preliminary results examining the design of a three component NS/MO/MOF catalyst that facilitate HER, with focus on limiting precious metal quantity, irradiation intensity and irradiation time to provide maximal H<sub>2</sub> evolution.

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## Affiliation

StFX University

# Synthesis of non-canonical amino acids to study wet adhesion by blue mussels

Jincheng Ren<sup>1</sup>, Layla Owens<sup>1</sup>, Zoë McNeil<sup>1</sup>, Alexander Baker<sup>1</sup>

<sup>1</sup>Dalhousie University

Biodegradable wet adhesives are important materials for use in biomedical applications, coatings, and labels to minimize the impact on the environment. Blue mussels form strong water-resistant adhesions to rocks in the ocean with a protein mixture containing mussel foot protein-5 (MFP-5). Studies indicate that MFP-5 adhesion is enabled through the incorporation of dihydroxyphenylalanine (DOPA), a non-canonical amino acid, which are formed from tyrosine residues. We hypothesize that it is possible to further enhance the adhesion strength of wild-type MFP-5 by incorporating other specially designed non-canonical amino acids. This research focuses on the synthesis of proteogenic amino acids with altered chemical structures emphasizing altered pKa values compared with their natural counterparts. The primary synthetic approach employed in this project focused on an Erlenmeyer-Plöchl azlactone route to amino acids, which included a reduction by hydrogenation, enzyme-mediated chiral resolution, and acid-catalyzed deprotection. Multiple synthetic intermediates have been successfully synthesized and isolated through flash chromatography, characterized using nuclear magnetic resonance and mass spectrometry. The second approach utilized a one-step Nickel and Iridium catalyzed metallophotoredox reaction to yield the protected non-canonical amino acids by a cross-coupling reaction. To study the impact of non-canonical amino acids on adhesion, we first focus on a fluorescent reporter system to monitor the incorporation of these molecules within proteins during ribosomal-mediated protein synthesis. Synthetic DNA sequences were designed and optimized for expression with *E. coli*. Constructs were amplified by polymerase chain reaction and evaluated by electrophoresis. Resulting DNA was used in cell-free protein expression reactions to produce Mefp-5 with prepared amino acid mixes monitored using fluorescence over 6 hours. We demonstrate the synthesis of many potential non-canonical amino acids along with a fluorescent assay to monitor their incorporation into proteins towards the discovery of sustainable wet adhesive proteins.

## Affiliation

Dalhousie University

# Remediation of Persistent Environmental Contaminants of Interest: An Enlightening Approach to Nitroaromatic Transformations

Leah Baylis<sup>1</sup>, Geniece Hallett-Tapley<sup>1</sup>

<sup>1</sup>StFX University

Canada is home to approximately one third of the world's fresh water. However, high pollution rates have rendered some of these reserves unsafe for human use. Nitroaromatic molecules have been listed high environmental priority given widespread use in pharmaceutical, pesticide and textile industries. Many of these, including 2,4-dinitrochlorobenzene (DNCB), are deemed toxic, mutagenic, and carcinogenic. DNCB remediation is often problematic given its high-water solubility, enabling its transfer through food chains, with traditional routes requiring costly adsorption techniques limit pollutant removal. As such, photocatalytic detoxification has recently gained traction in the environmental remediation industry, using light-activated solids.

The current approach will examine the ability of novel plasmonic metal nanomaterials to promote photoreduction of a series of nitroaromatic substrates to improve upon the efficiency and sustainability of DNCB remediation. Previous work has shown the versatility of palladium and gold nanoparticle/metal oxides (Pd/Au/MO) to promote reduction and oxidation of organic molecules, respectively [1-4]. Transition metal composites, themselves, are intriguing given their adsorption ability and aptitude for in situ reduction (through H<sub>2</sub>) under mild, alcohol conditions. The current contribution will discuss methods for nanocatalyst synthesis and optimization of the photoremediation methodology from the perspective of nanoparticle functionalization, light intensity and reaction time.

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## Affiliation

StFX University



# Towards the Synthesis and Reactivity of Planar Bismuth (III) Pincer Complexes

Tamina Kirsch<sup>1</sup>

<sup>1</sup>Dalhousie University

As previously reported by the Chitnis group, trianionic pincer ligands can be used to obtain T-shaped Bi(III) complexes.<sup>1</sup> The distortion from a pyramidal geometry to a planar environment around the bismuth centre leads to an accessible 6p LUMO orbital which can interact with Lewis bases. Those classes of planar Bi(III) pincer complexes exhibit high Lewis acidity and open up the window for interesting applications, for example in catalysis.<sup>2</sup>

One approach to modify the Lewis acidity of the bismuth centre is mesomeric tuning.<sup>3</sup> In the originally reported trianionic ligand, the central bismuth atom is bound to three nitrogen atoms. Replacement of one of the nitrogen atoms of the ligand with a weaker pi donor is projected to lead to an increased Lewis acidity of the complex due to a decreased occupancy of the 6p orbital. This can be achieved by either exchanging one of the nitrogen atoms with a carbon atom or by incorporating the lone pair of the central N atom into the pi bonding system of the ligand backbone, for example by using a pyrrole-based ligand framework.

Attempts towards the synthesis of these Bi(III) pincer ligands will be discussed and their unexpected reactivities will be highlighted.

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## Affiliation

Dalhousie University

# APTES-functionalized TiN Nanoparticles for Solar Driven CO<sub>2</sub> Capture

Dreenan Shea<sup>1</sup>, Mita Dasog<sup>1</sup>

<sup>1</sup>Dalhousie University

As the global climate crisis has become increasingly prevalent, the capture, storage and conversion of CO<sub>2</sub> has been at the forefront of industries worldwide.<sup>1</sup> Amongst shifting from fossil fuel to renewable energy techniques, trapping and controlled release of CO<sub>2</sub> has been an important topic of research.<sup>2</sup> Previously, amine scrubbing was the leading process for CO<sub>2</sub> cycling, however the use of high temperatures and toxic by-products in the regeneration process has led to the search of a better method.<sup>3</sup> Solid sorbents of basic nature have gained attraction for their use in carbon capture methods due to their binding efficiency and selectivity for weakly acidic CO<sub>2</sub>.<sup>4</sup> When compared to amine scrubbing, their incorporation into CO<sub>2</sub> cycling has decreased energy expenditure for regeneration. However, solid adsorbents still require high temperatures and therefore unsustainable heating practices with high-cost equipment.<sup>5</sup> To improve these shortcomings, plasmonic materials and their efficient light to heat conversion capabilities may be a viable substitute for electricity-based heating techniques.<sup>6</sup> Titanium nitride (TiN), an emerging plasmonic material, can convert sunlight to heat in a matter of nanoseconds,<sup>7</sup> facilitating low-energy, portable localized heat supply. The Dasog group has recently functionalized the surface of TiN with 3-Aminopropyltriethoxysilane (APTES), using a simple microwave reaction. As APTES contains a terminal amine group, it has been shown to have an adsorption affinity for CO<sub>2</sub>.<sup>4</sup> The use of a surface amine group for enhanced CO<sub>2</sub> adsorption and solar-driven photothermal heating for sorbent regeneration, shows potential for cost-effective, renewable CO<sub>2</sub> capture. This presentation highlights the thermal stability, and amine quantification of TiN-APTES. Preliminary results for CO<sub>2</sub> cycling capabilities of TiN-APTES will also be investigated.

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#### **Affiliation**

Dalhousie University

# Development and Application of a Semi-Automated System to Monitor the Solubility of Iron-Containing Atmospheric Aerosol Particles

Sarah Garrett<sup>1</sup>, Jenny P.S. Wong<sup>1</sup>

<sup>1</sup>Mount Allison University

The fraction of atmospheric water-soluble iron (WS-Fe), which has both global climate and human respiratory health implications, can be modulated by atmospheric reactions of iron-containing aerosol particles, particularly through acid-catalyzed solubilization. While previous research has focused on acid-catalyzed solubilization of iron in mineral dust and combustion particles, particles generated from brake wear have recently been suggested to be a significant source of atmospheric WS-Fe. Investigating the acid-catalyzed solubilization of iron has proven to be labour intensive, requiring frequent monitoring for up to one week to simulate the average atmospheric lifetime of aerosol particles. To streamline these experiments, a semi-automated system was developed to perform a colourimetric analysis to quantify and speciate WS-Fe. This system was used to investigate the WS-Fe produced from brake wear particles in hydrochloric acid and nitric acid. Characterization of the semi-automated system indicates that it performs the colourimetric analysis comparably to a manual approach while being less labour intensive. Although results showed that the different acids tested did not significantly influence the fraction of WS-Fe produced, evidence suggests that redox reactions, occurring only in nitric acid, influence the predominant oxidation state of the WS-Fe.

## Affiliation

Mount Allison University



# Towards a Bis(Iminophosphorano) Substituted 9,10-Antraquinone as a New High Voltage, Double Concerted Active Material for Symmetric ORFBs

Nicholas Stevenson-Garagan<sup>1</sup>, C. Adam Dyker<sup>1</sup>

<sup>1</sup>University of New Brunswick

Addressing escalating energy demands and growing environmental concerns of CO<sub>2</sub> emissions, a shift from fossil fuels to renewable energy sources such as solar, wind, and hydroelectric energy is essential. Since these energy sources are intermittent, large-scale energy storage is required to effectively integrate them into the electrical grid. A promising technology for this are organic redox flow batteries (ORFBs), which use organic molecules as active material rather than metals found in traditional batteries. Current ORFBs have limitations in terms of energy density and are based on active materials that undergo only single electron processes. This work aims to develop a high voltage, concerted two-electron (two electrons added or removed at the same time and voltage) bipolar (three total redox states) active material using the 9,10-anthraquinone scaffold for a non-aqueous symmetric ORFB. To this end, the substitution reactions with tricyclohexyliminophosphorane (Cy<sub>3</sub>PNH) and 1,4-bis(tosyl)-9,10-anthraquinone were investigated. Though with NMR spectroscopy it revealed that the di-substituted product was not forming, so efforts were made towards the synthesis of the mono-substituted product. The resulting precipitate revealed the possible formation of an anthraquinone anion, rather than the desired mono-substituted product. This lead to further investigation of the solid and solution through 2D NMR spectroscopy and LC-MS, to better understand the product formation of this substitution reaction.

## Affiliation

University of New Brunswick

# $\alpha$ -Ketene substituted tetrylenes - A series of bifunctional main group complexes

Leif Kelling<sup>1</sup>, Viktoria Gessner<sup>1</sup>

<sup>1</sup>Ruhr-University Bochum

Over the last 50 years the development of low valent main group chemistry grew from a niche to a mature field in inorganic chemistry. Main group compounds that feature a lone pair and a vacant orbital were found to imitate the reactivity of transition metals and therefore gained big attention for the activation of small molecules, such as H<sub>2</sub>, CO, CO<sub>2</sub> and NH<sub>3</sub>.<sup>[1]</sup> One of the most studied compound class in this regard are tetrylenes, the heavier analogues of carbenes.<sup>[2]</sup> Tetrylenes generally favor the singlet ground state, whereby the position of HOMO and LUMO are dictated by the attached ligands.<sup>[3]</sup> This makes the heavier carbene analogues excellent candidates for mimicking transition metal reactivities. Amongst the rich variety of substituents, nitrogen based donors were found to be of high value for tetrylene stabilization. The ligand gained even more attention with the introduction of *N,N*-chelating ligands by Power<sup>[4]</sup> and the development by Roesky *et al*<sup>[5]</sup>. Latter one reported the synthesis of strained  $k^2$ -amidato substituted chloro-tetrylenes which since then functions as one of the most versatile precursor class in main group chemistry.

Recently, we reported the transition metal-free synthesis of ketenyl anions.<sup>[6]</sup> The strong carbon nucleophiles were shown to be versatile precursors for substitution reactions. Thereby, the usually unstable ketene function can readily be introduced into various electrophiles.<sup>[7]</sup> In this study we report the first series of  $\alpha$ -ketene substituted tetrylenes. Structural determination of the bifunctional compounds by single crystal X-ray diffraction resulted in interesting differences depending on ligand substitution and choice of main group element.

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### **Affiliation**

Ruhr-University Bochum

# Exploring Chemical Sources of Diffuse Interstellar Bands Through Quantum Mechanics

Ailish Sullivan<sup>1</sup>, Halis Seuret<sup>1, 2</sup>, Emily Smith<sup>1</sup>, Fraser Smith<sup>3</sup>, Tiffany Fields<sup>3</sup>, Tina Harriott<sup>1</sup>, Daniel Majaess<sup>1</sup>, Lou Massa<sup>4</sup>, Chérif Matta<sup>1, 3, 5, 6</sup>

<sup>1</sup>Mount Saint Vincent University, <sup>2</sup>Autonomous University of Morelos States, <sup>3</sup>Saint Mary's University, <sup>4</sup>City University of New York, <sup>5</sup>Université Laval, <sup>6</sup>Dalhousie University

Diffuse Interstellar Bands (DIBs) have remained a mystery since their discovery over a century ago. Despite numerous attempts, there is yet to be an undisputed molecular source proposed for any of the 500+ unknown absorption features. This research uses a functional group approach to explore the chemical sources of the first discovered DIBs, 5780 Å and 5797 Å. A python script was created to calculate the vibrational energies from a predetermined family of potentially associated DIBs, and subsequently compared to molecular data for ~16,000 molecules contained within the RASCALL 1.0 database. Molecular candidates with vibrational energies consistent with 5780 Å contained a primary amide and a hydroxyl functional group. For 5797 Å, promising molecular candidates were some derivative of 2-cyclopenten-1-one. The proposed molecular candidates were validated using Monte Carlo simulations. Additionally, quantum mechanics calculations were performed using Gaussian 16 software to obtain the optical spectra of each candidate in the 5797 Å family. First, the geometry of the four candidate molecules was optimized at the MP2/aug-cc-pVTZ level of theory to ensure minimums in the potential energy surface. The optical spectra were then computed using TD-DFT theory with three XC functionals: wb97x-D, PBE0, and CAM-B3LYP. Unexpected results for neutral molecules prompted the exploration of ionized molecules. Methods were repeated for +1/-1 and +2/-2 ions of each molecular candidate. Results showed promising indications that the molecular sources of the DIB families may be negatively charged species.

## Affiliation

Mount Saint Vincent University

# An N-H insertion reaction to prepare an $\alpha$ -phosphenium cation

Mitchell Baker<sup>1</sup>

<sup>1</sup>Saint Mary's University

$\alpha$ -Cationic phosphines have received considerable attention for their utility in a variety of catalytic reactions. As part of an undergraduate research project, we have been exploring the syntheses of such species through N-H insertion reactions with the phosphoazonium ion [Mes\*NP]<sup>+</sup>. When [Mes\*NP]<sup>+</sup> was treated with an equimolar amount of NacNac-H a single product was isolated. The solid was characterized spectroscopically and crystallographically and identified as the  $\alpha$ -cationic phosphine shown in the figure below. Other products obtained from related addition reactions and how they relate to previous literature reports will also be discussed.

## Affiliation

Saint Mary's University

# Synthesis and Redox Properties of Homoleptic Indium *o*-Amidophenolates

Suhjung Chun<sup>1</sup>, Glen Briand<sup>1</sup>, Tanner George<sup>2</sup>, Jason Masuda<sup>2</sup>, Gregory Sandala<sup>1</sup>

<sup>1</sup>Mount Allison University, <sup>2</sup>Saint Mary's University

Green Chemistry is the design of chemical products and process that reduce or eliminate hazardous substances in various aspects of chemistry [1]. Use of catalysts lowers the activation energy of the reaction, which increases the efficiency and reduces waste. Redox active catalysts commonly contain precious transition metals, which are expensive and toxic, but cheaper and environmentally benign metals such as indium can be used as greener alternatives [2]. Various indium compounds are commonly used as Lewis acid catalysts in organic syntheses. However, indium is predominantly stable in the +3 oxidation state, which makes it not ideal for redox catalysis. Through use of redox active ligands such as *o*-amidophenolates, indium complexes are potentially able to undergo reversible oxidation and reduction reactions without requiring the metal to undergo unfavourable changes in oxidation state [3]. The goal of this research is to synthesize homoleptic indium *o*-amidophenolate complexes and determine the reversibility of their chemical and electrochemical oxidation to gauge their potential utility as catalysts in chemical transformations.

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## Affiliation

Mount Allison University

# Photodecarboxylation of Phenylacetic Acid Derivatives

Joseph Nazak<sup>1</sup>, Matthew Lukeman<sup>1</sup>

<sup>1</sup>Acadia University

A common photochemical reaction of arylacetic acids is photodecarboxylation (PDC) to generate either radical or carbanion intermediates. For example, non-steroidal anti-inflammatory drug (NSAID) ketoprofen very efficiently undergoes PDC in aqueous solution ( $\Phi = 0.75$ ) to give a benzylic carbanion intermediate, a photoreaction that is ultimately responsible for skin blistering in patients exposed to UV irradiation. Phenylacetic acid derivatives are gaining interest for their potential in the design of photolabile protecting groups (PPGs) for the release of biologically active molecules. For this application, efficient photochemical cleavage without undesired side reactions is crucial. We have been investigating the photochemistry of a variety of substituted arylacetic acids in aqueous solution, and have found that the nature of the substituents play a critical role in reaction mechanism and efficiency, with electron-poor arylacetic acids undergoing PDC most efficiently.

## Affiliation

Acadia University

# Examining the Effects of Hydrophobic Counterions on CMC Values of a Common Anionic Surfactant

Allison Clark<sup>1</sup>

<sup>1</sup>St. Francis Xavier University

Micellar systems have many important commercial and industrial applications, including body washes and detergents, drug delivery systems, oil recovery, and soft-templating materials for nanoparticle synthesis, etc. Our lab has been investigating the presence of additional electrolytes or other surfactants in micellar systems which has significant effects on its physiochemical properties. Specifically, we have been examining the effects of various tetraalkylammonium salts on the critical micelle concentration (cmc) of a common anionic surfactant, sodium dodecyl sulfate (SDS). At a certain minimum surfactant concentration, monomers will spontaneously aggregate via self-assembly into micelles, and we define that concentration as the cmc. We obtained cmc values and the degrees of counterion dissociation ( $\alpha$ ) via conductance measurements. The mass transport of the hydrophobic and surfactant counterions were examined by diffusion measurements via NMR spectroscopy. The results are interpreted in terms of increasing counterion hydrophobicity which decreases the cmc values of the anionic micellar system.

## **Affiliation**

St. Francis Xavier University



# Dissolving Barriers in Chemical Detection: Navigating Electrochemical Surface-Enhanced Raman Spectroscopy (EC-SERS) Beyond Water

Isabela Drozdowski<sup>1</sup>, Christa Brosseau <sup>1</sup>

<sup>1</sup>Saint Mary's University

Non-aqueous electrochemical surface-enhanced Raman spectroscopy (EC-SERS) was shown to be a potentially useful and beneficial approach for the characterization and analysis of hydrophobic compounds. EC-SERS itself is a well-established spectroelectrochemical technique that is continuing to emerge and develop, but there is a shortage of non-aqueous work in the field. Continuing to adapt and modify the method is important for broadening the applications and benefits of EC-SERS. The technique starts with Raman spectroscopy, which measures inelastically scattered photons to generate a vibrational fingerprint of a molecule. However, the measured Raman signal is intrinsically weak, particularly when applied to a molecule in solution due to the minimal scattered photons. By using nanoscale metals which generate localized surface plasmon resonance (LSPR) when struck by an incident beam, the Raman signal is enhanced, constituting surface-enhanced Raman spectroscopy. Electrochemistry furthers this enhancement, by drawing analyte closer to the surface through an applied potential. EC-SERS has been routinely used for aqueous analyte solutions. Lesser discussed is EC-SERS in non-aqueous solvents, likely due to the strong Raman signal associated with organic solvents, and the unfamiliarity surrounding non-aqueous electrochemistry. Non-aqueous EC-SERS has various advantages, including being relatively inexpensive, it can study species with wide ranging solubility, and it makes use of reusable screen-printed electrode (SPE) sensors. Despite these benefits, there are also obvious limitations to the method, such as the potential for unexpected solvent interactions, as well as interference from organic solvent and non-aqueous electrolyte which may prevent low levels of detection. To observe solvent interactions, and to establish and validate non-aqueous method, 2,2'-bipyridine, a classic EC-SERS system was studied in both methanol and acetonitrile. Meanwhile, to assess limitations associated with interference, to demonstrate the enhancing ability of the system, and to address possible future avenues for this research, bisphenols A (BPA) and bisphenol S (BPS) were studied using the non-aqueous EC-SERS method.

## **Affiliation**

Saint Mary's University

# Decoding Nature's Medicine: Method Development for the Analysis of Traditional Mi'kmaq Birch Bark Extract by Two-Dimensional Liquid Chromatography (2D-LC)

Rachael Ball<sup>1</sup>, Christa Brosseau<sup>1</sup>, Matthias Bierenstiel<sup>2,3</sup>, Vlada Zuieva<sup>3</sup>, Patricia Granados<sup>1</sup>

<sup>1</sup>Saint Mary's University, <sup>2</sup>Maskwiomin, <sup>3</sup>Cape Breton University

Birch Bark Extract (maskwio'mi) is a natural product that has been traditionally prepared by the Mi'kmaq people for thousands of years. This extract continues to be exploited today for its various medicinal properties. Despite longstanding knowledge of using birch bark extract to treat a variety of skin conditions, the active ingredient in this mixture has yet to be identified. To identify the active ingredient(s), it is crucial that a highly sensitive and selective separation technique be developed, to isolate components of this very complex mixture. In collaboration with local Mi'kmaq skincare company Maskwiomin, this research highlights the development of a multiple heart-cutting two-dimensional liquid chromatography (2D-LC) method for the separation and qualitative analysis of components in birch bark extract. 2D-LC is an extremely powerful and promising analytical technique for the separation of complex mixtures, as it allows select <sup>1</sup>D peaks to be subsequently analyzed using ideally orthogonal chromatographic <sup>2</sup>D parameters for further separation. 10 major component peaks, as well as 2 internal standard peaks from the birch bark extract's <sup>1</sup>D chromatogram, were selectively analyzed and optimized by multiple heart-cutting in the second dimension of the 2D-LC. To allow for future mass spectrometry analysis of extract components, a <sup>2</sup>D fraction collection method was optimized. Using this method, the 12 studied fractions were able to be isolated and stored for further analysis. Future work involves continuing to analyze the isolated <sup>2</sup>D fractions by mass spectrometry, with the goal of identifying the compounds responsible for the healing properties of birch bark extract.

## Affiliation

Saint Mary's University

# Ketoanilides as Surrogates for Electrophiles as well as Nucleophiles

Aditya Vardhan<sup>1</sup>, Oliver Cail<sup>1</sup>, Amitabh Jha<sup>1</sup>

<sup>1</sup>Acadia University

Certain ketoanilides and their analogues demonstrate significant utility as precursors for decorated *N*-acyliminium ions (electrophiles) and cyclic tertiary enamides (electron-rich alkene/nucleophiles). This characteristic of ketoanilides can be leveraged in synthesizing alkaloid-like polyheterocycles by employing suitable reaction partners. In one pursuit, ketoanilides derived from 2-acetylbenzoic acids underwent reactions with Betti bases, yielding spiro benzo[*f*]chromeneisoindolinones. This reaction is facilitated by the inverse electron demand hetero-Diels Alder reaction between cyclic tertiary enamides generated from ketoanilide and *o*-quinone methide produced from the Betti bases. Furthermore, these ketoanilides readily form *N*-acyliminium ions under the influence of Lewis/Bronsted acids, resulting in facile electrophilic aromatic substitution products on electron-rich aromatics such as indoles. Ketoanilides derived from 2-acetylbenzoic acid and levulinic acid also underwent facile self-coupling via inverse electron demand hetero-Diels Alder reaction in the presence of Lewis/Bronsted acids, involving *N*-acyliminium ions and cyclic tertiary enamides formed *in situ* from the same ketoanilides. Representative products obtained in this endeavour are depicted in the accompanying figure.

## Affiliation

Acadia University

# I'm Blue (da ba dee da ba di): Synthesis of Pyrimidine-Based TADF Emitters

Robert Horne<sup>1</sup>, Barry A. Blight<sup>1</sup>

<sup>1</sup>University of New Brunswick

Organic Light Emitting Diodes (OLEDs) provide our electronic displays with high contrast, energetically efficient emission that allows for the high-definition images expected from modern technology. Blue emitters for these devices are challenging from a synthetic and energetic perspective, which will be discussed. In recent years, thermally activated delayed fluorescence (TADF) has been of great interest in material science. These organic compounds display high outputs of visible light while also eliminating the need for heavy metals typically used in devices, making these emitters fantastic OLED candidates. I will present our progress towards pyrimidine-based deep blue emitters which utilize electron donor-acceptor pairs to take advantage of TADF for OLED materials. In achieving this, we will see an increase in colour saturation of the deep blue visible region, while decreasing overall energy consumption of every day devices.

## **Affiliation**

University of New Brunswick

# Synthesis of PSiP-Nickel Complexes with a Reduced Steric Profile for Application in Alkene Hydrogenation and Selective Isomerization-Hydroboration Catalysis

Jay Tang<sup>1</sup>, Laura Turculet<sup>1</sup>

<sup>1</sup>Dalhousie University

The development of Earth-abundant transition metal (e.g., Co, Fe, Ni) catalysts for chemical synthesis is key to fostering sustainability in the chemical industry and represents an important contribution to the development of clean technology and manufacturing. Such catalysts are necessary for the industrial-scale synthesis of pharmaceuticals and fine chemicals (e.g., fragrances, flavorings, agrochemicals). These processes currently use scarce platinum group metal catalysts (e.g., Rh, Ir, Pd, and Pt) that are obtained via energy-intensive mining and extraction leading to a high carbon footprint and are thus not compatible with current sustainability goals. In this context, the Turculet group has pursued the development of multidentate ligands featuring a silyl donor that can function as a hydride reservoir in the metal coordination sphere, as such metal-silyl cooperativity can facilitate the desired catalytic reactivity.<sup>1-3</sup> This presentation focuses on the synthesis and coordination chemistry of a new tridentate bis(phosphino)silyl (PSiP) ligand derivative that features a reduced steric profile compared to our previously established work. The utility of such bis(phosphino)silyl Ni species in hydroboration and hydrogenation catalysis featuring a broad range of substrates, such as aliphatic alkenes and styrene derivatives, will also be described.

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## Affiliation

Dalhousie University

# Leveraging Secondary Coordination Sphere Lewis Acid Inclusion on PCP Pincer Frameworks for Metal Ligand Cooperative Bond Activation

Ali Nasoudi<sup>1</sup>, Marissa Clapson<sup>1</sup>

<sup>1</sup>UPEI

Chemistry is experiencing a call to action concerning the development and implementation of sustainable chemical processes and transformations.<sup>1</sup> The development of base metal catalysts, in place of their precious metal counterparts, is one method to reduce both cost and toxicity while opening avenues for novel reactivity.<sup>2</sup> In recent years, pincer complexes have shown remarkable catalytic activity.<sup>3</sup> Milstein et al. provide excellent examples of metal ligand cooperation utilizing the secondary coordination sphere utilizing pyridine and acridine-based ligands which undergo an aromatization/de-aromatization sequence during bond activation.<sup>4</sup> Looking to further take advantage of the secondary coordination sphere, recent research has focused on the inclusion of Lewis basic and acid moieties into the ligand periphery as a means to tailor reactivity.<sup>5</sup> Herein, we describe preliminary results in the synthesis of a series of PCP pincer ligands featuring silyl moieties in the secondary coordination sphere for applications in catalytic esterification of carboxylic acids and alcohols. The formation of strong Si-O bonding interactions are leveraged to activate the carboxylate functionally, alongside  $\pi$ -bonding interactions with the base metal center. Insights into the sustainability of the resulting complexes are provided through a truncated life cycle analysis.

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**Affiliation**

University of Prince Edward Island

# Sonochemical *N*-demethylation of Alkaloids

Liah Christie<sup>1</sup>

<sup>1</sup>Saint Mary's University

## Sonochemical *N*-demethylation of Alkaloids

Liah D. Christie, and Robert D. Singer

Department of Chemistry

[liah.christie@smu.ca](mailto:liah.christie@smu.ca)

Saint Mary's University

Halifax NS B3H 3C3

The opioid crisis in North America is a rampant and detrimental issue, the impact of which is felt at all levels of society. Access to efficient, inexpensive, and environmentally conscious routes to life-saving pharmaceuticals such as Naloxone and Naltrexone are essential tools for combating both acute toxicity and long-term dependence in persons experiencing opiate addiction.

A critical step in the synthesis of the above pharmaceuticals is the selective *N*-demethylation of tertiary amines present in naturally occurring alkaloid precursors, allowing for the installation of different moieties as required in various Active Pharmaceutical Ingredients (APIs). Previous methodologies developed in the Singer group include the use of green solvents, Iron (0) Nanoparticles, and Liquid Assisted Grinding (LAG) to catalyze the *N*-demethylation of an array of *N*-methyl alkaloids. Our research focuses specifically on the *N*-demethylation step of a series of *N*-methylated alkaloids, including the precursors for Naloxone and Naltrexone.

Current work is directed at the use of sonochemistry as an alternative means to facilitate the *N*-demethylation reaction. Sonochemistry refers to the use of ultrasonic waves to enhance or alter the reactivity of a chemical reaction. In an effort to promote the 12 Principles of Green Chemistry, studies have been conducted in which the solvent, catalyst, various sonochemical parameters, and reaction time were altered. Additionally, the energy consumption of conventional heating, mechanochemical, and sonochemical methodologies have been compared and are presented.

### **Affiliation**

Saint Mary's University



# Metabolic biomarkers of neurodegeneration in a novel mouse model

Sophie Kieffe<sup>1</sup>, Drew Locke<sup>1</sup>, Grace Mercer<sup>1</sup>, Haley Adams<sup>1</sup>, Lindsay Cahill<sup>1</sup>

<sup>1</sup>Memorial University of Newfoundland

The brain is one of the most metabolically active organs and healthy brain metabolism is critical for normal memory and cognitive function. Recent evidence suggests a link between metabolic dysfunction and neurodegenerative diseases such as Alzheimer's disease (AD). While it is challenging to determine molecular and cellular mechanisms that precede the onset of AD in humans, animal models provide an opportunity to directly study the disease pathophysiology. This study aims to study brain metabolism throughout disease progression in a novel mouse model that reproduces several clinical features of AD.

Brain tissue samples were collected from the decrepit mouse model of neurodegeneration (a spontaneous mutation in a mitochondrial-associated gene) from 50 days (before disease onset) to 150 days (premature death). Healthy controls were included. Metabolite profiles were determined using <sup>1</sup>H high-resolution magic angle spinning magnetic resonance spectroscopy on a Bruker 600 MHz spectrometer with a 3.2 mm MAS solid-state NMR probe. Data was analyzed using MestReNova.

We investigated whether metabolites differed between five anatomical regions of the brain. We will also present preliminary results demonstrating changes in the metabolite profiles in the decrepit and control mice over their lifetime. The study demonstrates the promise of NMR metabolomics to study brain health.

## Affiliation

Memorial University of Newfoundland

# A Concerted Two-electron Bipolar Bispyridinylidene for Higher Voltage Symmetric, Organic Redox Flow Batteries

Eve Lavers<sup>1</sup>, Sydney Crain<sup>1</sup>, C. Adam Dyker<sup>1</sup>

<sup>1</sup>University of New Brunswick

Redox flow batteries (RFBs) are electrochemical storage devices that are a scalable system designed for large-scale applications. New research aims to develop a more sustainable and cheaper approach with non-aqueous solvents and organic active materials, where the use of organic solvents allows for higher cell voltages and higher energy density in the system. Along with using different solvents, symmetric redox flow batteries have been targeted with a single parent molecule that acts both as the catholyte and anolyte material. In this poster a new bispyridinylidene (BPY) compound BPYA<sub>5</sub> is shown to undergo the simultaneous two-electron oxidation and reduction processes for the symmetric non-aqueous RFB design. This simultaneous two-electron transfer makes this a desirable compound for high-capacity energy storage. The average cell potential of 1.31V in DMF with TBAPF<sub>6</sub> and 1.17V in LiTFSI, as salts, respectively represent improvements over previous work in the area.

## Affiliation

University of New Brunswick

# Preparation and monitoring of bifunctionalized gold nanorods via ligand exchange

Nghi (Lisa) La<sup>1</sup>, Hannah Cameron<sup>1</sup>, M.-Vicki Meli<sup>1</sup>

<sup>1</sup>Mount Allison University

Gold nanorods (AuNRs) are attractive for applications in detection and spectroscopy due to their unique plasmonic properties and tunable morphology. Further control and enhancement of AuNRs' plasmonic performance can be achieved through modification of their surface chemistry via ligand exchange. However, flexible ligand exchange on AuNRs is a challenge due to the cetyltrimethylammonium bromide (CTAB) bilayer structure on synthesized AuNRs that acts as both steric and electronic hindrance to incoming ligands. In this study, poly(ethylene glycol) 2-mercaptoethyl ether acetic acid thiol (PEG-COOH) was employed to displace CTAB on AuNRs using a direct ligand exchange procedure. This exchange occurred in Tris buffer at pH 3.0 with 0.3% SDS. The synthesized PEGylated AuNRs were characterized using UV-vis spectroscopy, zeta potential, ATR FT-IR spectroscopy, and Surface Enhanced Raman Spectroscopy (SERS), all of which confirmed successful PEG functionalization of AuNRs with only bromide residues. Further ligand exchange on the synthesized PEGylated AuNRs using 4-aminothiophenol (4-ATP) was conducted with real-time monitoring using SERS. Monitoring the ligand exchange process for the first 6 hours revealed an increase in 4-ATP signal in the first 2 hours, followed by a decrease in signal after the 2-hour mark. Further investigation is required to understand the decrease in signal observed, but this demonstrated the potential of SERS to be applied for real-time ligand exchange monitoring.

## **Affiliation**

Mount Allison University

# Synthesis and Reactivity of New Phosphino(silyl) Nickel Complexes for Application in Alkene Hydrogenation Catalysis

Tyler Saunders<sup>1</sup>, Laura Turculet<sup>1</sup>

<sup>1</sup>Dalhousie University

Research in the Turculet group targets the development of Earth-abundant 3d-transition metal complexes supported by multidentate (phosphino)silyl ligation for application in the catalytic hydrofunctionalization of unsaturated substrates such as alkenes, alkynes, and carbonyl derivatives.<sup>1-3</sup> In an effort to tune such catalysts and access increasingly reactive systems we have recently begun to explore the roles of coordinative unsaturation at the metal center and ancillary ligand steric features on reactivity.<sup>4</sup> In this regard, this presentation will detail the synthesis of new phosphino(silyl) ligand derivatives and our investigation of Ni coordination chemistry. The utility of such phosphino(silyl) Ni species in hydrogenation catalysis of sterically hindered alkenes will also be described.

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## Affiliation

Dalhousie University

# Isolating Hydroxyapatite from Atlantic Salmon Processing Waste - Transforming Trash to Treasure!

Sarah Boudreau<sup>1</sup>, Sabahudin Hrapovic<sup>2</sup>, Yali Liu<sup>2</sup>, Alfred Leung<sup>2</sup>, Edmond Lam<sup>2</sup>, Fabrice Berrué<sup>2</sup>, Francesca Kerton<sup>1</sup>

<sup>1</sup>Memorial University of Newfoundland, <sup>2</sup>National Research Council of Canada

The need for protein is increasing exponentially with the global human population, resulting in a large amount of waste being produced by the food processing industries. The demand for fish is higher than ever and there is a need for a solution for the ongoing waste management issues surrounding the disposal of by-products, including bones - a potential feedstock for hydroxyapatite. Hydroxyapatite,  $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ , is a versatile mineral that has been used in biomedicine, environmental remediation, and catalysis. Because of its value, it has previously been isolated from fish waste, however the methods described in literature are far too hazardous for industrial purposes. For example, some processes use temperatures up to 1,200 °C and/or concentrated bases (e.g., 50% NaOH). To overcome this challenge, we developed an industrially applicable method to isolate collagen-containing hydroxyapatite from Atlantic salmon (*Salmo salar*) waste using a cocktail of a protease and lipase. The enzymatic treatment was optimized using Design of Experiment and the parameters were evaluated using a 2<sup>4</sup> factorial design. Characterization techniques (e.g., infrared spectroscopy and x-ray diffraction), weight loss calculations, and thermogravimetric analyses were used to determine if an experiment would be considered a success or a failure. It was determined that a successful treatment only requires 15 µL g<sup>-1</sup> Neutrase and 7.5 µL g<sup>-1</sup> Lipozyme CALB L in 40 °C tap water for 6 h. To validate our method for industrial application, we successfully isolated >100 g of hydroxyapatite by treating 15 salmon frames (backbones) simultaneously, and we demonstrated our method is less impactful than others by doing a simplified gate-to-gate life cycle analysis. The treatment described could potentially be a part of the solution to a core industry challenge of whole-fish utilization for increased revenue generation. Ongoing research into developing a top-down process to synthesize hydroxyapatite nanoparticles from the cleaned bones will be briefly discussed.

## Affiliation

Memorial University of Newfoundland

# Adapting Titration Experiments for Students with Colour-Vision Deficiencies

Erin Wiggins<sup>1</sup>

<sup>1</sup>Mount Saint Vincent University

This project finds a solution to a very prominent issue for colour-vision deficient students looking to pursue chemistry. In particular, chemistry uses lots of colour changing, or qualitative, experiments in the lab. For students who cannot see these colour changes, it becomes necessary for them to rely on lab mates and can no longer be independent in the lab. Using the mobile app 'Colour Blind Pal', which identifies the colour detected via a camera lens, students can participate equally in the lab with, or without, full colour vision.

## **Affiliation**

Mount Saint Vincent University

# Journey Through Crystallography

Tanner George<sup>1</sup>, Jason Masuda<sup>1</sup>

<sup>1</sup>Saint Mary's University

In keeping with the theme of the conference, I want to discuss how learning crystallography has been the single most important thing that has happened to me as a scientist, enabling me to come full circle with a life-long fascination with crystals in the natural world and throughout a number of video games growing up. Single crystal X-ray crystallography enables the identification and quantification of the contents within a crystal, and in personal experience, this technique enables the best understanding of what exactly is happening in the endless crystals synthetic chemists produce, when other methods like UV-Vis, Infrared, and Nuclear Magnetic Resonance fail. Crystallography underpins our understanding of life via elucidation of DNA, B12, ribosomes, and a slew of other biological receptors, while simultaneously being the reason chemists and geologists know so much about the periodic table from widespread materials and most minerals. I strongly feel the reason crystallography is not more popular is simply because very few people are aware of its power from a young age, as I only truly realized its potential when I was in my third year of university when I learned SMU is the leader in crystallography output in the Atlantic provinces, and 6 years later I am proud to be a part of that output with 38 published crystal structures, and around 3-5x as many ready for review when their respective publications are completed both internal to SMU and external including University of New Brunswick, Dalhousie, Mount Allison, Saint Francis Xavier, Carlton, and Crandall universities.

## **Affiliation**

Saint Mary's University

# Acaricidal Effects of Encapsulated Thymol Nanoparticles, Thymol Microemulsions, and Synergistic Agents on the American Dog Tick, *Dermacentor variabilis* (Say) (Acari: Ixodidae)

Adrien Nette<sup>1</sup>, Dr. Nicoletta Faraone<sup>1</sup>

<sup>1</sup>Acadia University

Due to rising global temperatures, tick populations are growing and extending to northern regions. As consequence, zoonotic tick-borne diseases are increasing in prevalence all around the world and are likely to lead to an escalating global health risk. As the incidence of these tick-borne diseases increase, so has the dependence on synthetic tick repellents and acaricides. In recent years, there has been a growing demand for plant essential oil (EO) pest management products because they are relatively safe and environmentally friendly. However, EO compounds lack environmental persistency and have low aqueous solubility. Therefore, encapsulation with wall materials is used to protect, slow the release of, and increase solubility of EO compounds. Another way to improve the efficacy of EOs is by combination with a synergistic compound. Piperonyl butoxide (PBO) is a commonly used synthetic insecticide synergist. Piperine is a natural compound that has similar structural features to PBO and may exert similar synergistic activity. In this work, the acaricidal effects on adult female *Dermacentor variabilis* ticks of unencapsulated thymol (main component in white thyme, *Thymus zygis*) were compared with the acaricidal effects of thymol gum Arabic nanoparticles (GA NPs), a thymol soybean oil in water (O/W) microemulsion, and a [10:1] [PBO:thymol] mixture. It was determined that the LC<sub>50</sub> of thymol was 4.78 mg mL<sup>-1</sup> (95% CI: 3.85 - 5.71) 96 hours post-exposure. The encapsulation efficiencies of thymol and piperine in the GA NPs were low, ranging from 12.0 to 37%, and 9 to 23%, respectively. Despite this, the GA NPs had significantly greater acaricidal activity than unencapsulated thymol at a comparable concentration, resulting in 76% mortality 168 hours post-exposure. Therefore, encapsulating thymol in GA NPs is a promising method for delivering the active compound to ticks for future development of an acaricidal product. The encapsulation efficiency of thymol in the soybean O/W microemulsion was assumed to be 100%. However, the soybean O/W microemulsion had significantly less acaricidal activity than unencapsulated thymol at a similar concentration. The emulsion only resulted in 40% mortality 168 hours post-exposure, possibly due to the large particle size which may limit surface interactions with the ticks. The [10:1] [PBO:thymol] mixture had antagonistic acaricidal effects instead of synergistic. Investigations of different concentrations of the PBO and thymol mixture may improve the synergistic activity. Attempts to encapsulate piperine in GA NPs, a beta-cyclodextrin physical mixture, and zein encapsulations had very poor encapsulation efficiencies and were not evaluated further or used for acaricidal testing.

## Affiliation

Acadia University



# Novel Redox-active Functional Groups Exploiting the $\alpha$ -Effect

Anas Iqelan<sup>1</sup>, Andrew Grant<sup>1</sup>

<sup>1</sup>Mount Allison University

The Grant Lab recently disclosed the development of a novel class of redox-active materials based on the redox behavior of the 2,5-dithio-7-azabicyclo[2.2.1]heptane ring system<sup>1</sup>). These materials are being examined for applications in green gold mining, redox-flow batteries, and anti-viral PPE. This Poster describes our attempts to increase the reduction potential of these materials by taking advantage of the  $\alpha$ -effect. We describe our attempts at synthesizing several 2,5-dithio-7-azabicyclo[2.2.1]heptane ring systems that have an R-O- or an R-N- attached to the bridgehead nitrogen. These compounds have proven difficult to synthesize.

1) Redox Active Materials, Processes and Uses Thereof: US Patent 11,851,444B2

## **Affiliation**

Mount Allison University

# Novel Acrylamide Michael Acceptors

Tiana Sharpe<sup>1</sup>, Andrew Grant<sup>1</sup>

<sup>1</sup>Mount Allison University

Compounds possessing Michael accepting properties have gained considerable attention in anti-cancer drug discovery owing to their ability to form covalent bonds with biological enzymes. The inclusion of an enone functional group is required to facilitate these Michael addition reactions. This study proposes the development of novel dihydrothiophene-based acid chloride (1). Acid chloride (1) is expected to react with a variety of primary and secondary amines to produce novel acrylamide-like Michael acceptors. This talk will describe the successful synthesis and characterization of this novel acid chloride and demonstrate its inherent versatility. Utilizing the acid chloride, the dihydrothiophene modification was successfully appended to three different amines, yielding three novel acrylamide-like Michael acceptors. Preliminary testing of their ability to act as Michael acceptors has proven to be unsuccessful thus far.

## **Affiliation**

Mount Allison University

# Fluorescence-based studies on host-guest inclusion complexes of modified $\beta$ -cyclodextrin with anilinonaphthalene sulfonates

Justine Guidon<sup>1</sup>, Brian Wagner<sup>1</sup>

<sup>1</sup>University of Prince Edward Island

Host-guest inclusion is an important field in supramolecular chemistry. It is driven by noncovalent interactions between a host and a guest molecule resulting in an inclusion complex in which a guest molecule enters the cavity of a macrocyclic host molecule. Fluorescence spectroscopy is one of the techniques used to study host-guest chemistry as a change in the emission intensity or wavelength maximum can be observed from the host-guest interaction. Such change can be quantified and analyzed by calculating the binding constant,  $K$ . The binding constant indicates the stability of the host-guest complex and how favourable the equilibrium process is. This work focuses on performing fluorescence-based thermodynamic studies using a modified  $\beta$ -cyclodextrin as the host and anilinonaphthalene sulfonates as the guests. Thermodynamic studies offer crucial information on the fundamental understanding of the complexation process such as obtaining the enthalpy and entropy of inclusion. In order to perform a thermodynamic study, both the host and guest molecules are required to be pure and homogenous. Modified cyclodextrin are of interest as they are known to improve the host properties such as increasing the solubility and the fluorescent enhancement of the guest creating a stronger inclusion compared to their corresponding unmodified cyclodextrins. However, modified cyclodextrin are often non-homogenous as they have different pattern of substitution. One commercially available homogenous modified cyclodextrin is 2,6-di-O-methyl- $\beta$ -cyclodextrin. This host was chosen to perform fluorescence-based thermodynamic studies with different anilinonaphthalene sulfonates to compare the change in the strength of the inclusion between the different guests molecules. This poster will present the results of the thermodynamic studies of 2,6-TNS and 2,6-ANS with 2,6-di-O-methyl- $\beta$ -cyclodextrin including the enthalpy and entropy of inclusion.

## Affiliation

University of Prince Edward Island

# Fluorescence-Based Studies of the Host-Guest Inclusion of 6-anilinonaphthalene-2-sulfonic acid (2,6-ANS) by a Water-soluble Pillar[5]arene

Emma Ramsay<sup>1</sup>, Brian Wagner<sup>1</sup>

<sup>1</sup>University of Prince Edward Island

Pillar[n]arenes are a relatively new class of macrocycle, composed of a number (denoted by n) of substituted phenyl rings, linked by methylene bridges in the para position. They are of particular interest for host-guest inclusion studies, in which a smaller guest molecule is held within the internal cavity of a host molecule, in this case a pillar[5]arene, by non-covalent interactions. The assembly of these complexes can be analyzed using fluorescence spectroscopy.

Non-water-soluble pillar[n]arenes are commercially available and have been studied in our research group in the past, but their water-soluble counterparts must be synthesized. The overall goal of this project is to successfully synthesize a water-soluble pillar[5]arene and to perform fluorescence-based studies on its host inclusion abilities using 2,6-ANS and 1,8-ANS as the guest molecules. This will be done by measuring the fluorescence enhancement or suppression of the host-guest inclusion complex. From this data, the binding constant K will be extracted. A new water-soluble pillar[5]arene has been successfully synthesized using a modified literature procedure and has demonstrated a strong fluorescence enhancement of 2,6-ANS. Initial investigations into the binding characteristics of this new pillararene will be presented and analyzed.

## Affiliation

University of Prince Edward Island

# Exploring the Structure and Substrate Specificity of N-Methyltransferase 4 in *Catharanthus roseus* via Molecular Operating Environment (MOE)

Daniel Deschênes<sup>1</sup>, Ghislain Deslongchamps<sup>1</sup>

<sup>1</sup>University of New Brunswick

N-methyltransferases (NMTs) are essential enzymes in plant secondary metabolism, catalyzing the methylation of diverse substrates, some of which include monoterpenoid indole alkaloids (MIAs). *Catharanthus roseus*, a well-established model for studying MIA biosynthesis, produces many valuable MIAs with medicinal properties. This study used a computational approach to investigate the 3D structure and substrate specificity of a particular enzyme, CrNMT4, that uses the essential cofactor, S-adenosylmethionine (SAM), for methylating its substrate. A homology model of CrNMT4 was first constructed from its amino acid sequence using the Molecular Operating Environment (MOE), a drug discovery software platform. Using MOE, SAM was then submitted to molecular docking procedures to place the cofactor in the active site of the CrNMT4 enzyme. The complete catalytic model of CrNMT4 (with bound SAM) was then the target of docking experiments with various MIAs present in *C. roseus*, including strictamine, perivine, picrinine, norajmaline, ajmaline, and 3-hydroxytabersonine. Analysis of the docking scores as well as consideration of the geometric requirements for N-methylating the substrates with enzyme-bound SAM, suggested potential CrNMT4 activity toward some of the investigated MIAs. In particular, perivine exhibited a favorable binding geometry for N-methylation within the enzyme's active site. An independent LC-MS/MS analysis of the products generated by incubating CrNMT4 with perivine as the substrate confirmed its N-methylation to form the MIA, vobasine, thus demonstrating enzymatic N-methylation of perivine *in vitro*. The results also suggest that CrNMT4 may exhibit some methylation activity towards ajmaline, norajmaline, and 3-hydroxytabersonine. These findings provide compelling evidence for CrNMT4's involvement in the MIA biosynthetic pathways of *C. roseus*.

## Affiliation

University of New Brunswick

# **Microbial Impact on Wine: A Study of L'Acadie Vineyards Natural Wine**

Lo Grant<sup>1</sup>, Clarissa Sit<sup>1</sup>

<sup>1</sup>Saint Marys University

The Nova Scotia wine economy has an economic impact of \$254.3 million annually. L'Acadie Vineyards is an award-winning vineyard in Nova Scotia that produces natural wine from L'Acadie Blanc grapes. Natural wines rely on yeasts and bacteria present on the grapes at the time of harvest for the fermentation. This contrasts conventional wines where starter cultures are added to grape juice to initiate the fermentation. Due to the spontaneous nature of natural wine production, the microorganisms impacting the wine profile are unknown. To determine what yeasts and bacteria are impacting the wine, grapes were sampled for microbial isolation during the 2019, 2020, and 2021 harvests. DNA identification of isolated microbes is ongoing. Microbes known to impact wine fermentation will be used for in-lab fermentation of L'Acadie Blanc grape juice. Chemical analysis of L'Acadie Vineyards wine and in-lab fermented grape juice will be used to determine which isolated microbes may be impacting the wine profile. Chemical analysis will be conducted using hydrophilic liquid interaction chromatography (HILIC) coupled with mass spectroscopy. Major sensory compounds known to impact wine sensory profiles will be prioritized for identification and quantification. These compounds include sugars, organic acids, and other sensory compounds such as higher alcohols and esters. This project will benefit L'Acadie Vineyards by determining what is impacting their wine and how individual microbes impact the wine. Comparison of the 2019, 2020, and 2021 vintages will show how the chemical profile of their product is changing over time and if there is a resident microbial population impacting the wine each year. Broader impacts on the Nova Scotia wine economy are also possible. Isolated yeasts found to benefit the sensory profile of wine could be marketed as yeast starters.

## **Affiliation**

Saint Marys University

# Isolation of MIA Compounds in the Leaves of *Tabernaemontana divaricata*

Allyson Paul<sup>1</sup>

<sup>1</sup>University of New Brunswick

*Tabernaemontana divaricata*, commonly referred to as the pinwheel flower, is medicinal plant in the Apocynaceae family native to Asia. It is rich in monoterpenoid indole alkaloids (MIAs), many of which are used clinically for their anticancer, analgesic, and antioxidant properties. The botanical preparation is also used to help with different ailments such as inflammation, toothaches, and ocular problems. To further understand the elusive biosynthetic pathways for many MIAs in this plant, I attempted to purify and identify MIAs from the crude alkaloid extraction of 200 grams of leaves. I purified one MIA by thin layer chromatography (TLC), and determined its structure to be mehranine by liquid chromatography mass spectrometry (LC-MS) and 1D/2D Nuclear Magnetic Resonance (NMR) analyses.

## **Affiliation**

University of New Brunswick

# Concerted Two-electron Bipolar Bispyridinylidenes for Symmetric, Organic Redox Flow Batteries

Sydney Crain<sup>1</sup>, C. Adam Dyker<sup>1</sup>, Eve Lavers<sup>1</sup>

<sup>1</sup>University of New Brunswick

Redox flow batteries (RFBs) are increasingly recognized as promising energy storage systems for large-scale applications, particularly useful in combating the unreliability of solar and wind power systems. The earliest RFBs were metal-based active materials such as vanadium electrolytes in an aqueous media, however concerns over low energy density, sustainability and cost have led to exploration of organic compounds as active materials in non-aqueous solvents with wider voltage windows. The use of symmetric designs, where a single redox active material serves as both catholyte and anolyte, has been particularly effective in reducing capacity degradation caused by active material crossover, a common issue in systems with distinct catholyte and anolyte materials. To achieve acceptable energy densities, systems that undergo multielectron redox events are most desirable. The Dyker group has introduced ester-substituted bispyridinylidenes (BPYs) for symmetric non-aqueous organic redox flow batteries, which uniquely enable simultaneous two-electron oxidation and two-electron reduction processes at 1.01 V for higher-capacity storage. To enhance cell voltage, which is essential for practical energy densities, this work focuses on synthesizing, characterizing, and evaluating the stability and solubility of new BPY derivatives. These BPYs operate at higher and lower redox potentials, while maintaining efficient two-electron processes.

## Affiliation

University of New Brunswick



# Evaluating Embedding Space Representations of Sn2 Reactions Generated by Deep Tensor Neural Networks

Stefano De Castro<sup>1</sup>

<sup>1</sup>University of New Brunswick

As research on and alongside machine learning models continues, the extent of these models' capabilities and understanding are the topic of much interest. In line with this, SchNet, a machine learning model used primarily for reliable predictive energy calculations of stable molecules, is one of many Deep Tensor Neural Networks (DTNNs) being explored.

Previous research has shown the possibility of versatile transferred knowledge within its architecture, so this project served to expand on that by modelling reactions and transition states.

In this vein, 22 Sn2 reactions from a larger set of 114 reactions were examined in SchNet. The Reactants, Transition States, and Products were plotted in a PCA graph that reduces the 128 dimensions of SchNet down to 2. Multiple hypotheses were tried and tested as this process was done.

Preliminary results gave an initial showing of promise with a reasonable outline of Sn2 reaction pathways present within SchNet's Embedding Space. This introduces a fascinating possibility of further mapping out other reactions and transition states and suggests that a reasonable pathway may be realized for each one within SchNet's Embedding Space.

As our understanding of SchNet and other DTNNs deepens, there is hope that we may become more familiar with the extent of their usages, making us more efficient in our usage of them in future chemical research.

## **Affiliation**

University of New Brunswick

# **Poly(B5AMA) embedded cellulose nanocrystal (CNC) composites as antimicrobial coatings**

Catherine Doyle<sup>1</sup>, Marya Ahmed<sup>1</sup>

<sup>1</sup>University of Prince Edward Island

Surface contamination by microbes is of particular concern in hospital settings and contaminated surfaces are a major source of hospital acquired infections. One of the primary methods to combat microbial contamination is surface decontamination using aseptic agents such as alcohols. Among the other techniques that are studied antimicrobial coatings are of particular interest. Antimicrobial coatings are made of a variety of materials including nanoparticles and antifouling polymers, which prevent microbial attachment. A promising antifouling polymer is poly(vitamin B5 analogous methacrylamide) (abbreviated poly(B5AMA)) which was recently developed in the Ahmed research group and is being explored for its antimicrobial and antifouling properties. However, polymers alone as antimicrobial polymeric coatings suffer from various drawbacks including fast degradation, damage, and surface exhaustion with time that cannot be detected by the naked eye. Combining polymers with stimuli responsive nanomaterials that can visually change color upon surface fouling can provide an excellent alternative in the development of next generation antifouling coatings. In an effort to achieve these advanced polymeric coatings that can sense bacterial contamination, this study focuses on producing stimuli responsive antimicrobial sprayable coatings by modifying cellulose nanocrystals (CNCs) with poly(B5AMA) to form nanocomposites, along with the incorporation of anthocyanin dye to provide pH responsiveness. pH responsiveness will allow for detection of coating contamination by microbes due to changes in pH caused by the metabolic products of bacteria. Our results thus far show successful production of the nanocomposites, and confirm the ability of the anthocyanin dye to detect bacterial contamination indicating that the novel coatings designed are capable of detecting bacterial contamination.

## **Affiliation**

University of Prince Edward Island

# Immunomodulatory Mechanisms of mCA4, a Synthetic Host Defense Peptide

Samin Jahan<sup>1</sup>, Marya Ahmed<sup>1</sup>

<sup>1</sup>university of prince edward island

Host defense peptides (HDPs), formerly known as antimicrobial peptides (AMPs), represent a group of essential compounds of innate immunity. These peptides can elicit strong anti-infective properties as well as immune regulation, ubiquitously present in all organisms. These small positively charged amphipathic cationic peptides possess diverse roles regarding regulating and modulating the immune system, namely chemotaxis, cell differentiation, and pro- and anti-inflammatory cytokine production, by activating various intracellular cell signaling pathways. The activation of these pathways by HDPs are documented to promote wound healing, and act as anticancer, and anti-infective therapeutic agents. This study aims to evaluate the immunomodulatory potential of HDP recently synthesized and characterized by the Ahmed group and was originally derived from chicken Angiogenin 4. Our experimental procedures involve the treatment of mouse macrophages with mini chicken Angiogenin 4 (termed as mCA- 4) and evaluation of cytokine secretion, and modulating of two well-known immunoregulatory pathways, namely nuclear factor kappa B (NF- $\kappa$ B) and Mitogen-activated protein kinase (MAPK) by Western blot analysis. Our data indicate that mCA-4 is a pro-inflammatory peptide and activates MAPK and NF- $\kappa$ B signaling pathways, resulting in the secretion of pro-inflammatory mediators, including IL-1 $\beta$ , NO, and TNF- $\alpha$ , in treated macrophages. Future investigations will involve the evaluation of other intracellular pathways that may be involved in immunomodulation by this peptide and identifying the critical pathways regulated by mCA4, providing valuable insights into its therapeutic potential.

## Affiliation

University of Prince Edward Island

# Substituting excess Li by Na in NMC 640 Li-excess materials

Ian Monchesky<sup>1</sup>, Divya Rathore<sup>1</sup>, Jeff Dahn<sup>1,2</sup>

<sup>1</sup>Department of Physics and Atmospheric Science, Dalhousie University, <sup>2</sup>Department of Chemistry, Dalhousie University

Cobalt has been a key component in lithium-ion batteries for several decades.<sup>1</sup> However, due to cobalt's low natural abundance,<sup>2</sup> there has been a growing body of research surrounding the replacement of cobalt with manganese and nickel in NMC cathodes. When cobalt is replaced with manganese, NMC cathodes tend to exhibit poor rate capability. The addition of Mn<sup>4+</sup> reduces Ni<sup>3+</sup> to Ni<sup>2+</sup>, which can occupy sites in the lithium layer and hinders Li<sup>+</sup> diffusivity.<sup>2</sup> To reduce this Ni-Li cation mixing, excess lithium can be incorporated into cobalt-free cathodes to improve diffusivity. However, due to the rising cost of lithium,<sup>3</sup> sodium's low valency and high abundance make it an appealing candidate to replace excess lithium. This study examines whether excess inactive lithium can be replaced by sodium in NMC 640 materials.

The positive electrode material Li<sub>1+x-y</sub>Na<sub>y</sub>[Ni<sub>0.6</sub>Mn<sub>0.4</sub>]<sub>1-x</sub>O<sub>2</sub> for 0 ≤ x ≤ 0.07, 0 ≤ y ≤ 0.07 was synthesized from a 10 μm Ni<sub>0.6</sub>Mn<sub>0.4</sub>(OH)<sub>2</sub> precursor at 900°C. SEM measurements showed that Na-doping had little effect on crystal morphology and primary particle size, while XRD measurements showed that Na-doping decreased Ni in the Li layer. This decrease in cation mixing is generally considered to be beneficial for electrochemical performance.

These materials were cycled in coin cells against a Li anode in the voltage range of 3.0 V to 4.4 V. First discharge capacities for C/20 cells were comparable for all Na materials, while C/5 cells showed decreasing first discharge capacities with increased doped-Na. This suggests that replacing excess Li by Na has a negative impact on the rate capability. Capacity retention also decreased with increased doped-Na. Thus, while the morphology and C/20 discharge capacities were comparable for all Na samples, cycling at higher rates has a detrimental effect on Na-doped materials.

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## Affiliation

Dalhousie University

# **A molecular design of the sensor platform for the detection of breast cancer biomarkers**

ALOYNA MENDONCE<sup>1</sup>, Chun Keat Khor<sup>1</sup>, Anna Ignaszak<sup>1</sup>

<sup>1</sup>University of New Brunswick

Aptasensors are cutting-edge biosensors that utilize aptamers, which are single-stranded DNA or RNA nucleic acids, as recognition elements to detect a wide range of target molecules with high specificity and sensitivity. These sensors operate on the principle of molecular recognition, where the aptamer selectively binds to the target analyte to induce a measurable signal change. This signal change can be transduced into a detectable output, such as electrical, optical, or electrochemical signals, allowing for rapid and precise detection of various targets, including proteins, enzymes, antibodies, and other biological indicators. Aptasensors hold immense promise in different fields, especially in medical diagnostics due to their versatility and sensitivity. In this project, we are using an aptamer to target molecules for the breast cancer protein HER2 (human epidermal growth factor receptor 2). The main goal of this project is to design an aptasensor that can detect HER2 breast cancer thereby making the process of diagnosis reliable and accurate.

## **Affiliation**

University of New Brunswick

# Purifying and Identifying Monoterpenoid Indole Alkaloids from stems of *Tabernaemontana elegans*

Destiny Njoku<sup>1</sup>

<sup>1</sup>University of New Brunswick

***Tabernaemontana elegans*, commonly known as the toad tree from the family Apocynaceae and native to eastern and southeastern Africa, offers a multitude of medicinal properties that have been used for generations in numerous tribes of Tanzania as a remedy for lung ailments, treating tuberculosis and as a clotting agent to stop bleeding—making it part of a large group of plant-produced natural products known as monoterpenoid indole alkaloids (MIA). Total alkaloids from *Tabernaemontana elegans* stems were prepared via acid-base extraction to remove any pigment compounds and unwanted impurities. Three MIAs were purified by thin layer chromatography (TLC). Their structures have been determined by Liquid Chromatography Mass Spectrometry (LC-MS) and Nuclear Magnetic Resonance (NMR) to be Vobasine, Tabernaemontanine, and Dregamine.**

## **Affiliation**

University of New Brunswick

# Synthesis and Characterization of Tantalum Ditelluride Single Crystals

Madeline Nowlan<sup>1</sup>, Jan-Hendrik Carroll-Pöhls<sup>1</sup>

<sup>1</sup>University of New Brunswick

**Synthesis and Characterization of Tantalum Ditelluride Single Crystals** *Madeline (Nicole) Nowlan, Jan-Hendrik Carroll-Pöhls*

In recent years, transition metal dichalcogenides (TMDCs) are attracting immense attention in various fields including the biomedical sector due to their extraordinary electrical, thermal, biological, and optical properties. The combination of those unique properties makes them a great candidate for photoacoustic tumor imaging and sustainable drug release. TMDCs have the chemical formula  $MX_2$  where M is a transition metal and X is a chalcogen and are considered as quantum materials - materials which cannot be described by classical approaches. In this study, TaTe<sub>2</sub> single crystals - a low-temperature superconductive TMDC - were investigated. The single crystals were synthesized using a chemical vapour transport in which iodine was chosen as a transport agent. The shape and size of the crystals are strongly dependent on the iodine content and hence, single crystals were grown with different iodine content. The purity of the crystals was confirmed using powder X-ray diffraction. Furthermore, scanning electron microscopy and energy dispersive X-ray spectroscopy were applied to explore the morphology and the composition of the crystals, respectively. More iodine caused a longer smoother structure, in contrast to less iodine which formed more spherical prickly structures. The electrical conduction was measured as a function of temperature from 2 K to 320 K. While previous reports have investigated the influence of external pressure on the superconductivity, the effect of magnetic field on the electrical properties were investigated at low temperature to investigate the electron transport and the superconductive properties for different grown single crystals. Furthermore, the TaTe<sub>2</sub> crystals were exfoliated to prepare nanolayers which can exhibit different electrical properties than the bulk samples. This study applies a novel approach to tune those properties while maintaining ambient pressure, improving biomedical and superconductivity properties

## **Affiliation**

University of New Brunswick



# Hafnium Diselenide: A Step Toward Solving the Energy Crisis

Brianna Aubé<sup>1</sup>, Jan-Hendrick Carroll-Pöhls<sup>1</sup>

<sup>1</sup>University of New Brunswick

## Hafnium Diselenide: A Step Toward Solving the Energy Crisis

*Brianna Aubé, Jan-Hendrik Carroll-Pöhls*

Transition metal dichalcogenides (TMDCs) have unique electrical and thermal properties which make them ideal candidates for the improvement of renewable energy materials. In particular, their properties can be tuned, which gives them a wide range of applications in the fields of photovoltaics and energy storage. TMDCs have the general chemical formula  $MX_2$ , where  $M$  is a transition metal and  $X$  is a chalcogen and a layered structure along the  $c$ -direction.

Hafnium diselenide ( $HfSe_2$ ) - a semiconducting transition metal dichalcogenide - was explored as its band gap is in an ideal range for photovoltaics. Previous study revealed that  $HfSe_2$  is an n-type semiconductor with a band gap of 1.1 - 1.3 eV. In the first step,  $HfSe_2$  polycrystalline samples were synthesized using a solid-state approach. The powder was used to grow single crystals using the chemical vapour transport method, with iodine as the transport agent. Powder X-ray diffraction determined the purity of the crystals and confirmed  $HfSe_2$  was successfully prepared. Further characterization of the samples included using scanning electron microscopy and energy dispersive X-ray spectroscopy of the single crystals to ascertain the morphology and composition of the crystals, respectively. Recent literature shows that exfoliation of TMDC into single layers from its 3D bulk structure is possible due to weak van der Waals forces between layers - improving properties and enabling tuning. Preliminary exfoliation of  $HfSe_2$  crystals indicates its promise to prepare large monolayers to tailor the electrical properties. Furthermore, the electrical properties were measured as a function of temperature, showing semiconducting behaviour. Due to its high purity and unique electronic properties,  $HfSe_2$  can significantly increase the efficiency of photovoltaic applications.

### Affiliation

University of New Brunswick

# Purification and Identification of Monoterpene Indole Alkaloids from *Luculia Pinceana*: Ajmalicine and Tetrahydroalstonine

Stephen Silliphant<sup>1</sup>

<sup>1</sup>University of New Brunswick Fredericton

Heteroyohimbine type monoterpene indole alkaloids (MIA) extracted from the plant *Luculia Pinceana*, ajmalicine and tetrahydroalstonine, were separated and purified using Thin Layer Chromatography (TLC). Alkaloids were identified through Liquid Chromatography-Mass Spectrometry (LC-MS), as well as <sup>1</sup>H and <sup>13</sup>C Nuclear Magnetic Resonance (NMR) spectra with associated literature values. Structural conformation was verified via analysis of 2D NMR spectra.

## **Affiliation**

University of New Brunswick Fredericton

# Computational Investigation of the Thermoelectric and Mechanical Properties in Topological Quantum Materials

Elham Rezaee<sup>1</sup>, Jan-Hendrik Carroll-Pöhls<sup>1</sup>

<sup>1</sup>University of New Brunswick

Over 60% of world's energy is transformed into the inaccessible form of heat. Thermoelectric (TE) materials offer a direct way to turn waste heat into electricity and are widely utilized in space satellites, automotive vehicles, and solar-powered TE generators. For highly efficient thermoelectrics, these materials require an efficient conversion of a temperature gradient into electricity and a low heat conduction to preserve the high temperature difference. As the electrical and thermal properties are often intertwined, the discovery and optimization of TE materials are time-consuming and challenging. In recent years, topological TE materials have received notable consideration. These materials act as insulators in their interior but conduct electricity on their surface. Due to this unique combination of structure and physical properties, the electrical and thermal properties can be independently optimized leading to better devices for converting heat into electricity.

In this presentation, the electronic, thermal, and mechanical properties of two topological TE compounds -  $VP_2$  and  $CaP_3$  - were computed using advanced first-principles calculations based on density functional theory (DFT). Three key properties are essential for commercial TE materials: mechanical stability, heat conversion into electricity, and the maintenance of a large temperature difference. In the first part, the electronic band structure including the density of states (DOS) were calculated, providing comprehensive insights into the materials' abilities to efficiently convert heat to electricity. Furthermore, the phonon dispersions were computed indicating that low phonon modes will result in low thermal conductivity for both compounds. In addition to the TE properties, a mechanical analysis was conducted revealing good mechanical strength and toughness ensuring long-term structural integrity. The computational TE and mechanical properties of  $VP_2$  and  $CaP_3$  are not only promising for TE conversion but also provide detailed understanding to guide the experimental studies.

## Affiliation

University of New Brunswick

# Comparative Analysis of Cuticular Compounds in *Ixodes scapularis* and *Dermacentor variabilis* Ticks

Carys McMurray<sup>1</sup>, Nicoletta Faraone<sup>1</sup>, N. Kirk Hillier<sup>1</sup>

<sup>1</sup>Acadia University

Ticks, and the pathogens they vector, are a quickly-growing public health issue in Canada due to changing climate conditions, and diseases like Lyme disease pose an appreciable threat to the health humans and animals. *Ixodes scapularis* and *Dermacentor variabilis* are two species of ticks commonly found in Canada that have the potential to vector serious illnesses, and both are increasing in population size and range. Despite this, not much research has investigated an important aspect of their biology - cuticular hydrocarbons. Analysis of cuticular compounds can be an incredibly useful tool for collecting physiological data about arthropods - cuticular composition can provide information about diet, environment, age, sex, infection status, mating status and more in insects, but this field is relatively untapped in ticks. This thesis aims to build a better understanding of how cuticular composition differs between these two species as well as within each species between different sexes, as well as in ticks infected with *Borrelia burgdorferi* bacteria. Cuticular compounds were extracted from individual ticks and analyzed by gas chromatography - mass spectrometry to identify differences in the composition of cuticular compounds. Tick extracts were also tested in behavioural bioassays to determine whether cuticular compounds may play a role in tick chemical communication. Notable differences were found in the cuticular profiles of the two different species when compared, as well as between males and females of the same species, though only minor differences were found between infected ticks and uninfected ticks. Tick cuticular extracts were not found to be attractive when tested in bioassays. This study offers new insight into the intra- and inter-species variation of cuticular compounds found in *I. scapularis* and *D. variabilis* ticks, as well as the effect of *Borrelia burgdorferi* bacteria on the tick cuticular composition.

## Affiliation

Acadia University

# Formulations to Deliver Cannabidiol and Psilocybin for the Treatment of Neuropsychiatric Disorders

Emily Sabean<sup>1</sup>, Nicoletta Faraone<sup>1</sup>

<sup>1</sup>Acadia University

Anxiety and depression are the two most common neuropsychiatric disorders worldwide, affecting an estimated 284- and 264-million people, respectively, as of 2018. The current medications available to treat these disorders have a low rate of response with numerous unpleasant side effects (i.e., heart problems, suicidal ideation, insomnia, memory loss). Despite this, very few new treatment options have come to the market in the last twenty years.

Cannabidiol (CBD) and psilocybin have both recently been investigated as potential treatment agents. CBD and psilocybin are both natural products of which research has shown promise for their use to treat several diseases. This project, developed in partnership with Halucenex Life Sciences Inc. (Windsor, NS, CA), aimed to formulate a drug delivery vehicle containing CBD, psilocybin, and a combination of the two using several emulsification and encapsulation techniques. The encapsulation of active ingredients in a suitable wall material allows for protection from degradation, enhances adsorption in the body, increases the stability and shelf-life of the product, and allows for a controlled release of the active pharmaceutical ingredients. The overall goal of this project was to determine if CBD and psilocybin could work synergistically - enhancing their beneficial effects.

Progesterone was used in preliminary experiments as a proxy for CBD, whereas 5-hydroxytryptophan (5-HTP) or tryptophan were used as proxies for psilocybin. The techniques explored included inverse gelation and external gelation, as well as powder complexes and Pickering emulsions. The original inverse gelation method was not successful, and thus no data is reported. A second version of the inverse gelation method, as well as the external gelation method, were successful and yielded gel-like spheres loaded with the active ingredient. The emulsions were analyzed to determine their zeta potential, size, and polydispersity index (PDI). The active ingredient was re-extracted from the gels and analyzed with High Performance Liquid Chromatography (HPLC) to determine their encapsulation efficiencies.

The most promising methods for each active pharmaceutical ingredient were determined to be (1) External Gelation for progesterone ( $EE\% = 33 \pm 5$ ), (2) Physical Mixture/External Gelation for CBD ( $EE\% = 48 \pm 10$ ), (3) UV for 5-HTP ( $EE\% = 42$ ), (4) UV for tryptophan ( $EE\% = 1.4 \pm 0.3$ ), and (5) [5:5] [EMULSION:ALGINATE] for the double encapsulation of CBD and tryptophan ( $EE\% = 61 \pm 8$ ). This suggests that the combination of these active ingredients may be enhancing their effects, but more studies are required to confirm.

## Affiliation

Acadia University

# Synthesis and Characterization of a New Pyrenoimidazole Based Organic Fluorophore - An Experimental and Computational Study

Nicholas Qiu<sup>1</sup>, Yuming Zhao<sup>2</sup>

<sup>1</sup>First Author, <sup>2</sup>Supervisor

Organic fluorophores hold promising applications in biomedicine, most notably for the development of numerous fluorescence imaging probes and photosensitizing agents used in photodynamic therapy [1]. This presentation describes the preparation of a new pyrenoimidazole-based organic fluorophore **2** through a metal hydride reduction of a previously synthesized organic fluorophore with a 6*H*-phenanthro[4,5-*cde*]pyreno[4',5':4,5]imidazo[1,2-*a*]-azepin-6-one core (**1**) by Shahrokhi and Zhao [2]. The synthetic conditions of **1** were first optimized to give a high yield of 87%, allowing **2** to be synthesized easily and at higher scales. Single crystals of **2** were successfully grown and subjected to X-ray single crystallographic analysis to understand its molecular structure and solid-state packing properties. UV-vis absorption and fluorescence spectroscopic analyses of fluorophore **2** show high fluorescence and acidochromic behavior in solution, as well as increased solubility in acidic conditions. Comparative studies on fluorophores **1** and **2** in terms of the degree of  $\pi$ -conjugation, intermolecular interactions, and electronic transitions were carried out with the aid of DFT and TDDFT calculations. Our results indicate that **2** can be used as an efficient and tuneable fluorophore in sensing and imaging applications.

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## Affiliation

Memorial University

# Impact of exposure to environmental pollutants on placental metabolism

Haley Adams<sup>1</sup>, Katherine Steeves<sup>1</sup>, Lindsay Cahill<sup>1</sup>

<sup>1</sup>Memorial University

**For a healthy pregnancy, the placenta needs to meet the metabolic demands of the fetus and supply it with sufficient oxygen and nutrients. Our group has recently shown using NMR-based metabolomics that genetic deficiency and environmental exposures can perturb the metabolic profile of the placenta, resulting in adverse pregnancy outcomes. This study aims to evaluate the effects of exposure to persistent organic pollutants, legacy and novel per- and polyfluoroalkyl substances (PFAS), on placental metabolism.**

**Placental tissue samples were collected from healthy control pregnant CD-1 mice and mice exposed to perfluorooctanoic acid and fluorotelomer ethoxylates throughout gestation. The tissue was flash frozen in liquid nitrogen and stored at -80°C. Metabolite profiles were determined using <sup>1</sup>H high-resolution magic angle spinning magnetic resonance spectroscopy on a Bruker 600 MHz spectrometer with a 3.2 mm MAS solid-state NMR probe. Data was analyzed using MestReNova and MetaboAnalyst.**

**The relative concentration of several metabolites that are essential nutrients for fetal development were found to be significantly altered in the PFAS-exposed groups. This study adds to the growing literature that has demonstrated the significant impact of environmental pollutants on placental function and emphasizes that efforts should be made to minimize exposure to pollutants during pregnancy.**

## **Affiliation**

Memorial University

# Investigating NO<sub>2</sub> Gas Adsorption and Reactivity in Zirconium-Cluster-Based MOFs Using Breakthrough Analysis

Mackenzie Reid-Hall<sup>1</sup>, Michael Katz<sup>1</sup>

<sup>1</sup>Memorial University of Newfoundland

Nitrogen oxides (NO<sub>x</sub>) form a class of environmental pollutants containing gaseous nitric oxide (NO) and nitrogen dioxide (NO<sub>2</sub>). These gases are a product of everyday combustion processes, and can have serious effects on human health and the environment. Additionally, NO<sub>x</sub> are capable of forming harmful secondary pollutants such as gaseous nitrous acid (HONO). Metal-organic frameworks (MOFs) are a type of porous material commonly used for gas capture and storage. In this talk, zirconium-cluster-based MOFs such as UiO-66, UiO-66-NH<sub>2</sub>, and UiO-66-[OH]<sub>2</sub> were investigated for their ability to react with NO<sub>x</sub> gases. An automated breakthrough analyzer (ABR) was used to do flow through experiments with 10% NO<sub>2</sub> in N<sub>2</sub> gas flowing through a packed column of MOF with a downstream mass spectrometer that gave real-time data for up to five gases over the course of the experiment. Experimental evidence supported that the reaction of NO<sub>2</sub> gas with the MOFs produced a NO<sup>+</sup> radical, that was stored inside the MOF after NO<sub>2</sub> gas breakthrough. Evidence of NO<sub>3</sub><sup>-</sup> and NO<sup>+</sup> was observed in all of the MOFs, but with UiO-66-[OH]<sub>2</sub> we noticed wildly different NO<sub>x</sub> behaviour consistent with the proton-coupled-electron transfer (PCET) to produce NO gas. The other MOFs appeared to modulate the amount of NO gas vs. NO<sub>2</sub> gas that was produced in the NO<sub>x</sub> gas cylinder.

## Affiliation

Memorial University of Newfoundland



# Sea-ing Things Differently: Analysis of Bio-active Carbohydrates in Brown Seaweed

A. Stephenson<sup>1</sup>, O.M. Wyper<sup>2</sup>, F.M. Kerton<sup>3</sup>

<sup>1</sup>Undergraduate Honours Student, <sup>2</sup>PhD Candidate, <sup>3</sup>Research Supervisor

Seaweed, also known as macroalgae, has been a valuable resource for decades, finding diverse applications in agrochemistry, cosmetics, and nutraceuticals. Recent advancements have highlighted its potential as a versatile material capable of capturing CO<sub>2</sub>, increasing its utilization in emerging fields such as dermatology and renewable energy. However, unlocking the full range of benefits from seaweed first requires an understanding of its composition.

Fucoidan, a sulfated polysaccharide abundant in seaweed, stands out as a promising biopolymer with various therapeutic properties, particularly in dermatological applications. Previous studies have indicated a positive correlation between the degree of sulfation in fucoidan and its dermatological activity, such as anti-inflammatory properties. In this study, the focus on fucoidan derived from *Laminaria digitata*, a native Newfoundland seaweed, revealed a substantial presence of sulfated fucoidan along with the identification of galactose, another unique sugar in fucoidan compared to others found commercially. To understand its properties, advanced analytical techniques such as Electrospray Ionization (ESI) coupled with Tandem MS (MS/MS) can be used to determine sulfate position. Along with sulfate position, other factors such as molecular weight are also able to be determined via matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-ToF MS), and GPC.

This proposes a biorefinery concept to maximize the utilization of seaweed biomass, aligning with circular economy principles outlined by the United Nations and the 12 Principles of Green Chemistry. By efficiently extracting valuable compounds like fucoidan for dermatological applications, while simultaneously repurposing the remaining seaweed biomass for energy production or other value-added products, sustainability and resource efficiency are maximized.

## Affiliation

Memorial University Of Newfoundland

# Chromium(III) Diamino-bis(phenolate) Catalysts for Ring-opening Copolymerization Reactions using Renewable Resources

Cyler Vos<sup>1</sup>, James Beament<sup>1</sup>, Aayush Anand<sup>1</sup>, Christopher Kozak<sup>1</sup>

<sup>1</sup>Memorial University of Newfoundland

We have previously reported the use of chromium(III) diamino-bis(phenolate) complexes as catalysts for ring opening polymerization (ROP) of epoxides and ring opening copolymerization (ROCOP) of epoxides and CO<sub>2</sub>. Our group's research now focuses on expanding the polymer classes that can be formed using these catalysts. This involves using different monomers, such as cyclic anhydrides and lactones, for incorporation into copolymers. The use of renewable resources to form these polymers in a sustainable manner is of growing importance as our world drives to maintain a circular economy, therefore the sustainable production of these polymers has been a focus of our research. These terpolymers incorporating CO<sub>2</sub>, epoxides, and other monomers into their structure can show tunable physical properties, having a wide range of molar masses and glass transition temperatures. The coordination geometry of the metal complex has shown to be important. The activity and selectivity for different monomers is influenced by whether a *trans*-ligand-inducing tetradentate diamino-bis(phenolate) ligand (ONNO) is used, or a tripodal diamino-bis(phenolate) ligand (O<sub>2</sub>NN') is used, which enforces a *cis*-ancillary ligand orientation. The influence of the ligand, choice of co-catalyst, catalyst loading, monomer-to-monomer ratio, and temperature will be discussed in this presentation, as well as the potential use of an additional renewable initiator to assist in less active copolymerization reactions giving rise to a larger array of polymers able to be produced efficiently in a sustainable manner.

## Affiliation

Memorial University of Newfoundland

